How to evaluate and publish Binary Phase Diagram Data

Best Practice Guidelines for Evaluation
&
Notes for Authors

3rd Edition, 2012

Authoring team: MSIT®

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P. Perrot, A. Pisch, P. Rogl, R. Schmid-Fetzer*

These guidelines give detailed instruction to those which want to contribute to the *MSIT® Binary 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® Binary Evaluation Program* these Notes for Authors are binding.

Critical Evaluation of Binary Phase Diagram Data

Best Practice Guidelines for Evaluation
&
Notes for Authors

Interested scientists are welcome to download and printout "Critical Evaluation of Binary 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/binary-evaluations/

In publications please refer to:

G. Cacciamani, G. Effenberg, R. Ferro, S. Ilyenko, P. Perrot, A. Pisch, P. Rogl, R. Schmid-Fetzer (Eds.), *Critical Evaluation of Binary Phase Diagram Data. Best Practice Guidelines for Evaluation & Notes for Authors. Edition 3*, MSI, Stuttgart (2012)

Introduction

The knowledge base *MSI Eureka* provide concise and consistent descriptions of 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 tables and text.

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.

Contents

MSIT

Chapter 1
Structure of a Binary System Report

Small system reports should not be split in chapters, whilst large system reports should be structured in the following chapters

Heading

Literature Data   *concise summary of other people's work*

Solid Phases

Phase Equilibria

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

Notes on Materials Properties and Applications

Miscellaneous

References

Tables

Figures

Topics without sufficient data are skipped.

1.0. Heading

<div style="border:1px solid">

25.02.12 Cu-Ti 1

Cu –Ti (Copper – Titanium)

Ibrahim Ansara , Volodymyr Ivanchenko, Vitaliy Dubenskiy

Literature Data

……………………

</div>

Please include page numbering on every page 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.

1.1. Literature Data

Gives a short overview of 'what has been done by whom'.

A brief review of the published works on the binary system should outline the experimental methods, the amount of work involved in studying the binary system and state the extent of agreement between different authors.

The arguments on which the decision on final selection of data will be based are NOT given here but later in the individual chapters.

Experimental methods used in investigation of the phase equilibria, crystal structure and properties should be described in Table 1: "Recent Investigations of the X-Y System". In the first column the reference is given; experimental techniques used are listed in the second column and in the third column temperature/composition/phase range studied should be given. See example system report on the Cu-Ti system ammended to the "Notes for Authors".

Note: thermodynamic studies also should be mentioned in the "Literature Data" section, however experimental details should not be given in Table 1, but in the corresponding tables of the "Thermodynamics" section.

If for the system a review or assessment is available which covers the earlier data, make a reference to this review in a following way "Literature data up to 1985 are given in the review by [1994Mur]. The X-Y system was subsequently studied by several techniques and for different temperature and composition ranges which are listed in Table 1." Then in Table 1 only publications after 1985 should be described.

Such a table is mandatory in each system report, where experimental information is given.

1.2. Solid Phases

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

The Table "Solid Phases" should incorporate **all** phases of the binary system, *starting* with unary, proceeding to binary. This includes crystalline, high pressure and metastable phases (indication about amorphous and glassy state could be given under "Miscellaneous").

For the unary phases it is recommended to use the data prepared by the MSIT Program Board. They are available on request from evaluation@msiport.com.

Each phase appears only once. If the phase fields show a continuous connection at any range of the phase diagram then this phase must be described as a single unique phase. See examples below in Cu-Ni and Fe-Si (with closed γ loop) systems. If the αFe and δFe solution ranges merge in the system, the designation of αδFe is recommended. Please report the maximum solubilities and the respective temperatures.

Different phases are separated by horizontal lines in the table.

Cu–Ni phase diagram (top):

- Temperature, °C (y-axis)
- Ni, at.% (x-axis), from Cu to Ni
- L
- 1455
- 1084.62
- (Cu,Ni)
- 354.5
- $\alpha_1 + \alpha_2$
- T_c
- 354.4

Fe–Si phase diagram (bottom):

- Temperature, °C (y-axis)
- Si, at.% (x-axis), from Fe to Si
- 1538
- 1394
- (γFe)
- 1410
- 1414
- 3.8
- ($\alpha\delta$Fe)
- α_1
- 1200
- 1212
- 1203
- β
- 1212
- 1220
- 1207
- ζ_α
- 1060
- 982
- 965
- η
- 937
- 912
- α_2
- 825
- 770
- ε
- ζ_β
- (Si)
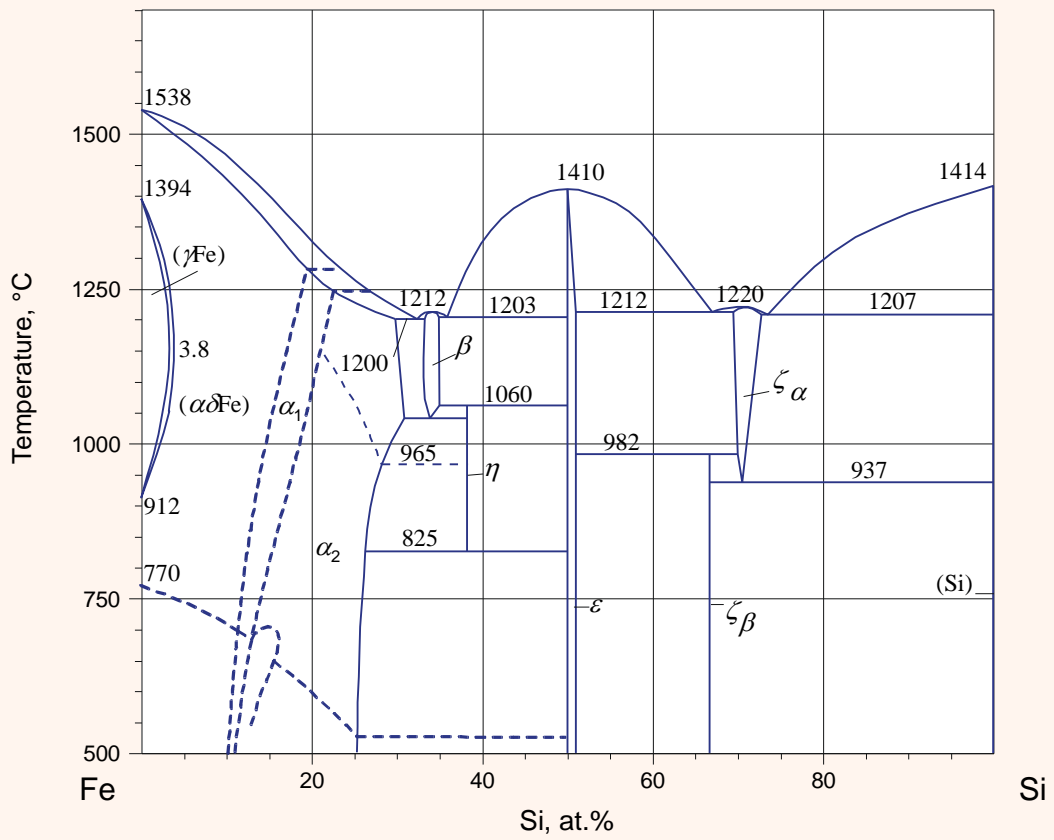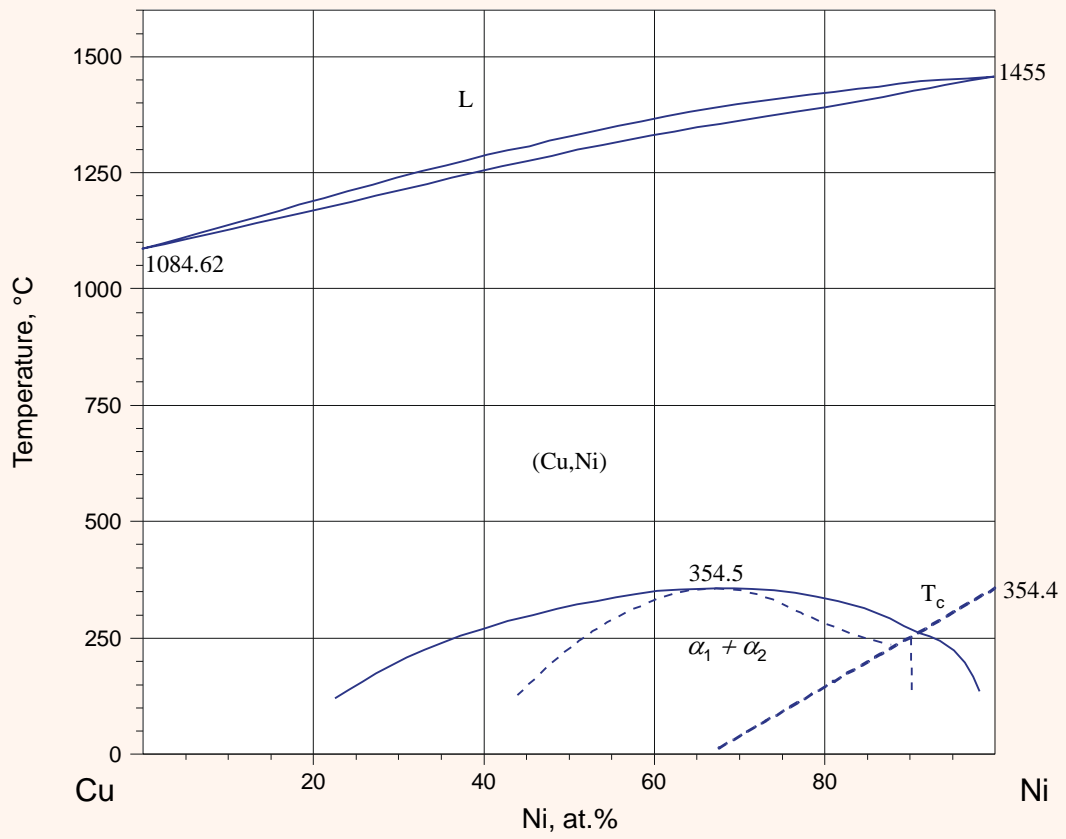
1. The *first column* of the table contains the formulae (at least an approximate one) of the phases. Whenever Greek letters are used to denote phases, these symbols must also appear in the first column.

Two phases must not have the same name and one phase can not have two different names. A one to one relationship 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 3.4. We use SiC (instead of CSi) in the C-Si system.

Different phases with the same formulae are distinguished by:

a. different symbols ε, ε', for allotropic transformations

b. Roman letters (I), (II), for pressure modifications

c. the temperature range of phase stability.

Different temperature modifications can be further indicated by lower case letters in brackets behind the phase designation, with

a. (h) = high temperature modification

b. (r) = room temperature modification

c. (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 $βPr_3Al_{11}$, αδFe are possible within one system report.

2. 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.

3. 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 :

$1\text{Å} = 0.1 \text{ nm} = 100 \text{ pm}$; $1 \text{ kX} = 1.00202\text{Å}$

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:

$a = 2a' \sin(α'/2)$

$c = a' \sqrt{3}\sqrt{1 + 2\cos α'}$

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The Pearson symbol *hR*... should show the number of atoms in the hexagonal unit cell, e.g. αSm : *hR*9 , but not *hR*3 with reference to the number, 3, of atoms contained in the primitive rhombohedral unit cell.

4. *Column four* allows the inclusion of additional information, such as: references, comments on accuracy, concentrations, etc. The source of data has to be referenced.

Authors should indicate whether the original work has truly proven the existence of a binary phase or merely the presence of a metastable phase.

Examples for Table Solid Phases

Table 2: Solid Phases

Phase/ Temperature Range (°C)	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters (pm)	Comments
(Mg) <650	$hP2$ $P6_3/mmc$ Mg	$a =$ 320.944 $c =$ 521.076 $a =$ 320.5 to 321.4 $c =$ 520.5 to 522.6	pure Mg at 25°C [V-C2, Mas2] dissolves 0.14 at.% La at 613°C [Mas2] 0 to 0.44 at.% La at 600°C [V-C2]
(γLa) 918-865	$cI2$ $Im\bar{3}m$ W	$a =$ 426	pure La at 887°C [V-C2] dissolves ~29 at.% Mg at 712°C [Mas2]
(βLa) 865-310	$cF4$ $Fm\bar{3}m$ Cu	$a =$ 529.1	[V-C2] dissolves 9.4 at.% Mg at 546°C [Mas2]
(αLa) <310	$hP4$ $P6_3/mmc$ αLa	$a =$ 377.0 $c =$ 1215.9	[V-C2, Mas2]
LaMg$_{12}$ <640	$oI338$ $Immm$ CeMg$_{12}$(II)	$a =$ 1033 to 1034 $b =$ 1033 to 1034 $c =$ 7749 to 7774	7.14-8.3 at.%La [Mas2] [1995Gio]
La$_2$Mg$_{17}$ <670	$hP38$ $P6_3/mmc$ Th$_2$Ni$_{17}$	$a =$ 1037 $c =$ 1024	at 10.53 at.% La [Mas2] [1995Gio]
La$_5$Mg$_{41}$ <670	$tI92$ $I4/m$ Ce$_5$Mg$_{41}$	$a =$ 1482.2 $c =$ 1046.8	[1995Gio]
LaMg$_3$ <798	$cF16$ $Fm\bar{3}m$ BiF$_3$	$a =$ 749.4±0.2 $a =$ 748.8 $a =$ 751.0	[V-C2, Mas2, 1995Gio] Mg-rich [1994Gio] La-rich (25 at.%La) [1994Gio]
LaMg$_2$ 775-725	$cF24$ $Fd\bar{3}m$ MgCu$_2$	$a =$ 877.4 $a =$ 880.1 to 880.6	[V-C2, Mas2] [1994Gio]
LaMg <745	$cP2$ $Pm\bar{3}m$ CsCl	$a =$ 397.0±0.3 $a =$ 396.2	[V-C2, Mas2]

* See page 10 for the instructions for creating overstrike characters

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1.3. Phase Equilibria

Show the accepted phase diagram. Do not describe this figure in the text. Unclear points may be commented here.

Invariant equilibria should be listed in Table "Invariant Equilibria" in sequential order by decreasing temperature. The basic principles are briefly outlined below.

Binary three-phase reactions

$L' \rightleftharpoons L'' + \alpha$ $L \rightleftharpoons \alpha + \beta$ $\alpha \rightleftharpoons L + \beta$ $\alpha \rightleftharpoons \beta + \gamma$ $\beta' \rightleftharpoons \alpha + \beta''$	monotectic reaction eutectic reaction catatectic 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"

To describe two-phase invariant equilibria the following terms can be used

Polymorph

Congruent

Critical point

Maximum (max_1, max_2)

Minimum   (max_1, min_2)

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. The reaction should be written:

L, α, β	d, degenerate

For a more detailed discussion of the treatment of degenerate reactions (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)

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Table 3: Invariant Equilibria
This section should include a table showing the details of the invariant equilibria present in the binary system; arrange with decreasing temperature. Four columns are necessary: reaction, temperature (°C), type, composition. For example:

Reaction	T (°C)	Type	Phase	Composition, at.%	
				Ti	Cu
L ⇌ Ti$_2$Cu	1012	congruent	L, Ti$_2$Cu	66.7	33.3
L ⇌ (βTi) + Ti$_2$Cu	1005	e$_1$, eutectic	L	70	30
			(βTi)	86.5	13.5
			Ti$_2$Cu	66.7	33.3
L ⇌ Ti$_2$Cu + TiCu	960	e$_2$, eutectic	L	57	43
			Ti$_2$Cu	66.7	33.3
			TiCu	52	48
L + TiCu ⇌ Ti$_3$Cu$_4$	925	p$_1$, peritectic	L	37.5	62.5
			TiCu	42.9	57.1
			Ti$_3$Cu$_4$	33.3	66.7

Note : use only **e$_i$ or p$_i$** for **three-phase equilibria**, decomposition- or formation-type, respectively:
e.g. e$_8$, monotectic; e$_9$, catatectic; e$_{10}$, monotectoid; p$_8$, syntectic

1.4. 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 (generaly 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 experimantal 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.
- For practical reasons, report only data published after 1989 at this stage
- 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:

"RTlnp_{O2} vs T"

or

"logp_{O2} 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 "RTlnp_{O2} vs T" is prefered.

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) ⇒ AB$_3$(s) }	25	ΔH = -11.2 ± 0.8	[1995Abc] dir.cal.
1/3 { A(α) + 2 B(β) ⇒ AB$_2$(s) }	25	ΔH = -17.8	[1996Mno] Calphad
1/3 { A(α) + 2 B(β) ⇒ AB$_2$ }	25 - 800	ΔG = -14.0 + 0.003 T	[1996Abc] derived from emf measurements
1/(2.56) { Ce + 1.56 Si ⇒ CeSi$_{1.56}$ }	800	ΔH = xxx	[1996Abx]
(1-x) A(L) + x B(L) ⇒ A$_{(1-x)}$B$_x$(L)	1000	ΔH = -15.0±1 -14.0±1	x= 0.3 x = 0.4 [1996Def] solution cal.
A(L) ⇒ L (n=∞, x_B=0.5)	1200	a_A = 0.5	[1994Ghi] emf
A(α, 25°C) + L(n=∞, 800°C) ⇒ L (x_B = 0.2, 800°C)	25 – 800	$\Delta H'_A$= 1.5±0.3	[1997Jkl] drop cal.
A(L) + L(n=∞) ⇒ L (x_B=0.2)	800	$\Delta H'_A$= -0.5±0.3	[1997Jkl] drop cal. H$_A$ (α⇒L) from [Din]
A(α, 25°C) + L(n=∞, 800°C) ⇒ L (x_B = 1, 800°C)	25 – 800	$\Delta H'_A$= 1.2±0.3	[1997Jkl] drop cal. Infinite dilution
½(H$_2$)(g) + L(n=∞) ⇒ 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 " $\overset{-\text{“}}{}$ " with the final editing.

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 ± 0.5 $S°$ = 38.9 ± 2.1	[1992Abc] DSC [1993Def] drop cal. (calculated from ΔH) [1998Ghi]
¼ AB$_3$	25 - 500	H(773)-H(298) = 12400 ± 500	[1995Jkl] drop cal.
α	25 - 500	H(773)-H(298) = 12800 ± 500	[1997Jkl] drop cal.

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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	$\log10(p_{B2}) = -4.5$	

General notes for the chapter "Themodynamics:

1) The authors should not give impression that thermodynamic data are evaluated here; just all data should be reported.
2) Graphical presentation of data is preferred.

1.5. Notes on Materials Properties and Applications

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

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

1.6. 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.

1.7. 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.

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The reference list should be written in the following style:

[2010Vog] Vogel, S., Stein, F., Palm, M., "Investigation of the Epsilon Phase in the Fe-Al System by High-Temperature Neutron Diffraction", *Appl. Phys. A*, **99**(3), 607-611 (2010), DOI: 10.1007/s00339-010-5619-y (Crys. Structure, Experimental, Phase Relations, 17)

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. Prop., 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, Phase Relations, #, 7)

Book:

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

Chapter of Book:

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

Proceedings:

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

If a reference is not available but quoted in a given literature or even in Chemical Abstract, 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) 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) quoted in C.A. 111-158477F

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

MSIT

Chapter 2
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.

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- 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 corrects published diagrams if necessary by redrawing according to theoretical rules (Gibbs phase rule, Schreinemakers rule, Gibbs-Konovalov rule, etc.).

- 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.

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

- Diagrams are the diagrams of the MSIT author(s).
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- 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.

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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

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

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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.

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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 3

Best Technical and Editorial Practice

3.1. Diagrams

The diagrams, which authors send to MSI will be digitized. The diagrams have to be as clear and complete as possible. Any error in these diagrams will enter the database. A correction at a later date is an avoidable, time consuming work that delays publication. Several points require special attention.

1. The diagrams have to be labelled 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 labelling has to occur in the units of the diagram itself.*

3. No general correction remarks should be included on the diagrams, e.g. "please change all liquidus curves to dashed": the diagram has to be redrawn by the author.

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

5. If *by exception* copies of diagrams from the literature are used as base drawing, these copies have to include the full description of the drawing:

a. continuous lines may not be interrupted due to low copying quality;

b. separated lines may not intersect or overlay;

c. The phase fields have to be re-labeled by the author according to the table "Solid Phases" after removing the original designations. Refrain from this approach and redraw the diagram if the readability becomes questionable!

6. If already digitized diagrams require corrections of line curvatures or angles between lines, these corrections have to be done with a *thin* pen, denoting clearly the correct location of the line.

7. Line styles and thickness:

Generally diagrams should be drawn by thin solid lines. Thin dashed lines are used to denote uncertainties. Thin dotted lines are used to show metastable equilibria. Thick dashed lines should be used for magnetic and second order transformations. Magnetic transformation should be marked by the "T_C", "T_N", or "T_m" labels.

8. Does the use of "after [xxxxAbc]" or "from [xxxxAbc]" in figure legends have any significance? If not, omit "after" and "from".

9. Always place references in square brackets [ ]; do not use anything else.

3.2. Text

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"; do not write "Ag_2Te-type" or "tie-line".

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

- The temperature symbol is written in italics: T, following the IUPAC.

- 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.

- 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. $L \rightleftharpoons (Te) + \mu$; **not** $L = (Te) + \mu$).

- 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. $L + (Ag, Au) \rightleftharpoons AuTe_2 + \gamma Ag_2Te$,

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

    $AuTe_2 + \gamma Ag_2Te$.

- There is a blank space before and after *equal, less than* and *more than* signs; *e.g.* $\kappa = 10$ and $0 \leq \kappa \leq 1$

- 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 $Co_2Ni(r)$.

Abbreviations

- An alloy may be abbreviated, for example, Cu-10Zn (at.%) or Ca-Mg50 (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.

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.%".
- Hours and days are abbreviated by h and d, respectively.
- Usually leave a space between a number and its unit (*e.g.* 0.28 eV, 260 h, 6.5 at.%, but between number and °C leave no blank, *e.g.* 286°C not 286 °C).

3.3. 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±3.

3.4. 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 - left side (element with lower Pettifor number); right side (element with higher 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	

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Chapter 4. Sample System Reports

Cu – Ti (Copper – Titanium)

Ibrahim Ansara, Volodymyr Ivanchenko, Vitaliy Dubenskiy

Literature Data

Literature data up to 1985 are given in the review by [1994Mur]. Subsequently the Cu-Ti system was studied by several techniques and for different temperature and composition ranges which are listed in Table 1. This system exhibits six intermetallic compounds Ti_2Cu, $TiCu$, Ti_3Cu_4, Ti_2Cu_3, $TiCu_2$ and $TiCu_4$ for which the structure and homogeneity ranges are fairly well established. $TiCu_4$ presents two polymorphs. However, there is considerable scatter in the reported phase boundaries.

In their study of the Cu-Fe-Ti system, [1994Ali] investigated the Ti_2Cu compound. The microstructure of the cast alloy contained only coarse grains with sharp boundaries, and the diffraction pattern only contained tetragonal structure of that compound.

[1996Oli] determined the structure, phases and kinetics of phase formation of the Cu-Ti by diffusion couple. In their examination they found all well known compounds except for Ti_3Cu_4 due probably to very slow kinetics of formation of that phase.

Several thermodynamic assessments were performed [1970Kau, 1978Kau, 1983Mur, 1985Sau, 1990Zen, 1991Zen]. In these studies, the stable phases Ti_2Cu_3 and $TiCu_2$ were not considered. Furthermore [1970Kau, 1978Kau] did not consider Ti_3Cu_4. In all these assessments, the non-stoichiometry of $TiCu$ and $TiCu_4$ was ignored. [1996Kum] reassessed thermodynamically the system, taking into account all the phases as well as considering the non-stoichiometry of $TiCu$ and $TiCu_4$. The calculated values of the enthalpy of formation of $TiCu$, Ti_3Cu_4, Ti_2Cu_3 and $TiCu_4$ are in excellent agreement with the values measured later by [1997Col] except for βTi_2Cu. However, the enthalpies of mixing of liquid alloys are more positive than those recalculated by [1982Kle].

Solid Phases

[1997Dur] determined the crystal structures of the Cu-Ti intermetallic phases in the samples annealed at 850°C. Their results agree perfectly well with [Mas2] assessment for that temperature.

[1999Nag] determined the lattice parameter of copper with titanium contents of 1.5, 3.0, 4.5 and 5.5 mass.% Ti, melted from an oxygen free copper and a Cu - 26 mass.% Ti master alloy and casted in a graphite mould. The samples were homogenized for 24 h at 850°C and then aged at 450°C for peak strength. The lattice parameter of the solution treated samples is linear with respect to x_{Ti} (Table 2). For the peak aged two-phase samples, the lattice parameter is equal to 362±5 pm. The value of 0.8 at.% Ti for the solvus at 450°C is obtained from this information.

Phase Equilibria

In accordance with [1994Ali] the thermal analysis of the alloy Ti_2Cu presented a single heat effect at 1012 ± 3°C. These results confirmed those obtained by [1966Ere] which would lead to a eutectic reaction L $\rightleftharpoons$ (βTi) + Ti_2Cu instead of a possible peritectic reaction as indicated in [1994Mur].

The assessed phase diagram is shown in Fig. 1 and is based on [1994Mur] with a modification of the Ti-rich region. Invariant equilibria in the Cu-Ti system are given in Table 3.

Thermodynamics

Enthalpies of formation of the intermetallic compounds Ti_2Cu, $TiCu$, Ti_3Cu_4, Ti_2Cu and $\beta TiCu_4$ were determined by solution calorimetry in liquid aluminium [1997Col]. The values are given in Table 4.

[1995Tur] determined the enthalpies of mixing of liquid copper alloys using a heat flux high temperature isoperibolic calorimeter. His results were then reported in a series of papers [1996Tur1, 1996Tur2, 1996Tur3, 1997Tur, 1998Tur1, 1998Tur2]. His values are more negative than those obtained by [1982Kle].

[1992Hos] measured at very dilute solution ($5 \cdot 10^{-6} < x_{Ti} < 3.4 \cdot 10^{-3}$) the activity of titanium by solid state emf measurements at 1373 K using oxygen sensor $ZrO_2(MgO)$ as solid electrolyte. [1999Pan] also measured the activity of titanium in the composition range 0.678-3.25 at.% and at 1423K by the same technique. The integral quantities reported do not extrapolate to zero at pure copper [1999Pan] and only the actually measured activity of titanium is given in Table 4. The reference state of solid titanium was not further specified. There is a significant difference with the assessed values from [1996Kum].

Notes on Materials Properties and Applications

Aged-hardening copper-titanium alloys by spinodal decomposition can be used for electric functional materials due to their high conductivity and strength.

These alloys show good glass forming tendency by rapid quenching from the liquid phase, the amorphizing range being wide due to very steep liquidus curves in the terminal regions and low melting compounds in its central region. A very shallow metastable liquidus curve is hence expected at low temperatures which would favor solid state amorphization.

Copper-titanium alloys are also used in the production of jet engines and gas turbines, while copper is added to Ni-Ti shape memory alloys to increase the strength differences between the parent and martensitic phases, and to improve the transformational cyclic behavior.

Miscellaneous

[1994Yam] determined the phase boundaries in the titanium-rich region under high pressure (1.9-2.8 GPa) on polished cylindrical samples serving as diffusion couples. The composition at the phase boundary (Ti)/(Ti)+Ti_2Cu was not affected by these high pressures. However the eutectoid temperature was lowered by about 16°C and the peritectic temperature L + (βTi) $\rightleftharpoons$ Ti_2Cu increased by about 50°C, the composition of copper in the (βTi) increasing by 4 at.%.

[1999Dob] used mechanical alloying under a pressure of 5GPa in order to synthesize 16 Cu-Ti alloys. They found that in the composition range 0-10 at.% Cu, the alloys were single supersaturated phases having the αTi (hexagonal) structure, while in the composition range 90-100 at.% Cu, the alloys were also single supersaturated phases with the αCu(fcc) structure. In the composition range 58-80 at.% Cu, mechanical alloying yielded amorphous structures.

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Table 1: Recent Investigations of the Cu-Ti System

Reference	Experimental Technique	Temperature/Composition/Phase Range Studied
[1994Yam]	EPMA	Ti-rich corner between 1000-1400 K
[1994Ali]	Diffusion couple, X-ray, Metallography	structure of diffusion zone
[1996Oli]	DTA, Hardness, X-ray, Metallography	structure and fusion of Ti_2Cu
[1999Nag]	X-ray	Cu-rich alloys and Cu-rich+$TiCu_2$ alloys

Table 2: Solid Phases

Phase / Temperature Range (°C)	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters (pm)	Comments
(Cu) < 1084.87	$cF4$ $Fm\bar{3}m$ Cu	$a =$ 361.46 $a =$ 361.47 + 33.38x_{Ti}	pure Cu at 25°C [Mas2] dissolves 8 at.% Ti at 885°C [Mas2] dissolves 0.8 at.% Ti at 450°C [1999Nag] 0<x_{Ti}<0.3646 [1999Nag]
(βTi) 1670-790	$cI2$ $Im\bar{3}m$ W	$a =$ 330.65	pure Ti(h) at 25°C [Mas2] dissolves 13.5 at.% Cu at 1005°C [Mas2]
(αTi) < 882	$hP2$ $P6_3/mmc$ Mg	$a =$ 295.06 $c =$ 468.35	pure Ti(r) at 25°C [Mas2] dissolves 1.6 at.% Cu at 790°C [Mas2]
Ti_2Cu < 1012	$tI6$ $I4/mmm$ $MoSi_2$	$a =$ 295.3 $c =$ 1073.4	[Mas2, V-C2, 1994Ali]
$TiCu$ < 982	$tP4$ $P4/nmm$ TiCu	a = 310.8 to 311.8 c = 588.7 to 592.1	48 to 52 at.% Cu [Mas2, V-C2]
Ti_3Cu_4 < 925	$tI14$ $I4/mmm$ Ti_3Cu_4	$a =$ 313.0 $c =$ 1994	[Mas2, V-C2]
Ti_2Cu_3 < 875	$tP10$ $P4/nmm$ Ti_2Cu_3	$a =$ 313 $c =$ 1395	[Mas2, V-C2]

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Phase / Temperature Range (°C)	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters (pm)	Comments
TiCu$_2$ 890-870	oC12 Amm2 VAu$_2$	a = 436.3 b = 797.7 c = 447.8	[Mas2, V-C2]
βTiCu$_4$ 885 - ≈400	oP20 Pnma ZrAu$_4$	a = 452.5 b = 434.1 c = 1295.3	~78 to ~80.9 at.% Cu [Mas2, V-C2]
αTiCu$_4$ < ≈ 500	tI10 I4/m MoNi$_4$		~78 to ~80.9 at.% Cu [Mas2]

Table 3: Invariant Equilibria

Reaction	T (°C)	Type	Phase	Composition, at.%	
				Ti	Cu
L ⇌ Ti$_2$Cu	1012	congruent	L, Ti$_2$Cu	66.7	33.3
L ⇌ (βTi) + Ti$_2$Cu	1005	e$_1$, eutectic	L (βTi) Ti$_2$Cu	70 86.5 66.7	30 13.5 33.3
L ⇌ TiCu	982	congruent	L, TiCu	50	50
L ⇌ Ti$_2$Cu + TiCu	960	e$_2$, eutectic	L Ti$_2$Cu TiCu	57 66.7 52	43 33.3 48
L + TiCu ⇌ Ti$_3$Cu$_4$	925	p$_1$, peritectic	L TiCu Ti$_3$Cu$_4$	37.5 42.9 33.3	62.5 57.1 66.7
L + Ti$_3$Cu$_4$ ⇌ TiCu$_2$	890	p$_2$, peritectic	L Ti$_3$Cu$_4$ TiCu$_2$	29 42.9 33.3	71 57.1 66.7
L + (Cu) ⇌ βTiCu$_4$	885	p$_3$, peritectic	L (Cu) βTiCu$_4$	23 8 19.1	77 92 80.9
Ti$_3$Cu$_4$ + TiCu$_2$ ⇌ Ti$_2$Cu$_3$	875	p$_4$, peritectoid	Ti$_3$Cu$_4$ TiCu$_2$ Ti$_2$Cu$_3$	42.9 33.3 40	57.1 66.7 60
L ⇌ TiCu$_2$ + βTiCu$_4$	875	e$_3$, eutectic	L TiCu$_2$ βTiCu$_4$	27 33.2 22	73 66.7 78
TiCu$_2$ ⇌ Ti$_2$Cu$_3$ + βTiCu$_4$	870	e$_4$, eutectoid	TiCu$_2$ Ti$_2$Cu$_3$ βTiCu$_4$	33.3 40 22	66.7 60 78
(βTi) ⇌ (αTi) + Ti$_2$Cu	790	e$_5$, eutectoid	(βTi) (αTi) Ti$_2$Cu	94,6 98.4 66.7	5.4 1.6 33.3
βTiCu$_4$ + (Cu) ⇌ αTiCu$_4$	~500	p$_5$, peritectoid	βTiCu$_4$ (Cu) αTiCu$_4$	~19.1 0.5 ~19.1	~80.9 99.5 ~80.9
βTiCu$_4$ ⇌ αTiCu$_4$ + Ti$_2$Cu$_3$	~400	e$_6$, eutectoid	βTiCu$_4$ αTiCu$_4$ Ti$_2$Cu$_3$	~22 ~22 40	~78 ~78 60

Table 4: Thermodynamic Data of Reaction or Transformation

| Reaction or Transformation	Temperature (°C)	Quantity per mol of atoms (kJ, mol, K)	Comments
$1/3\{\,2Ti(\alpha) + Cu(s) \Rightarrow Ti_2Cu\,\}$	25	$\Delta H = -8.6 \pm 1.6$	[1997Col] solution calorimetry
$\frac{1}{2}\{\,Ti(\alpha) + Cu(s) \Rightarrow TiCu\,\}$	25	$\Delta H = -11.1 \pm 1.7$	[1997Col] solution calorimetry
$1/7\{\,3Ti(\alpha) + 4Cu(s) \Rightarrow Ti_3Cu_4\}$	25	$\Delta H = -9.6 \pm 0.9$	[1997Col] solution calorimetry
$1/5\{\,2Ti(\alpha) + 3Cu(s) \Rightarrow Ti_2Cu_3\,\}$	25	$\Delta H = -9.4 \pm 1.3$	[1997Col] solution calorimetry
$1/5\{\,Ti(\alpha) + 4Cu(s) \Rightarrow TiCu_4\,\}$	25	$\Delta H = -5.5 \pm 1.1$	[1997Col] solution calorimetry
$Ti(s) + L(n=\infty) \Rightarrow L\,(x_{Ti})$ $0 \le x_{Ti} \le 0.0325$	1150	$\ln \gamma_{Ti} = -1.607 + 4.828\, x_{Ti}$	[1999Pan] emf, via oxygen activity
$Ti(L) + L(n=\infty) \Rightarrow L\,(x_{Ti})$ $0 \le x_{Ti} \le 0.7$	1600	$\Delta \overline{H}_{Ti} = (1 - x_{Ti})^2\,(-29.780 + 4.860 x_{Ti} - 142.990 x_{Ti}^2) \pm 2\sigma$	[1997Tur] solution calorimetry $2\sigma = \pm 0.1\;(x=0.1)$ $2\sigma = \pm 3.5\;(x=0.7)$
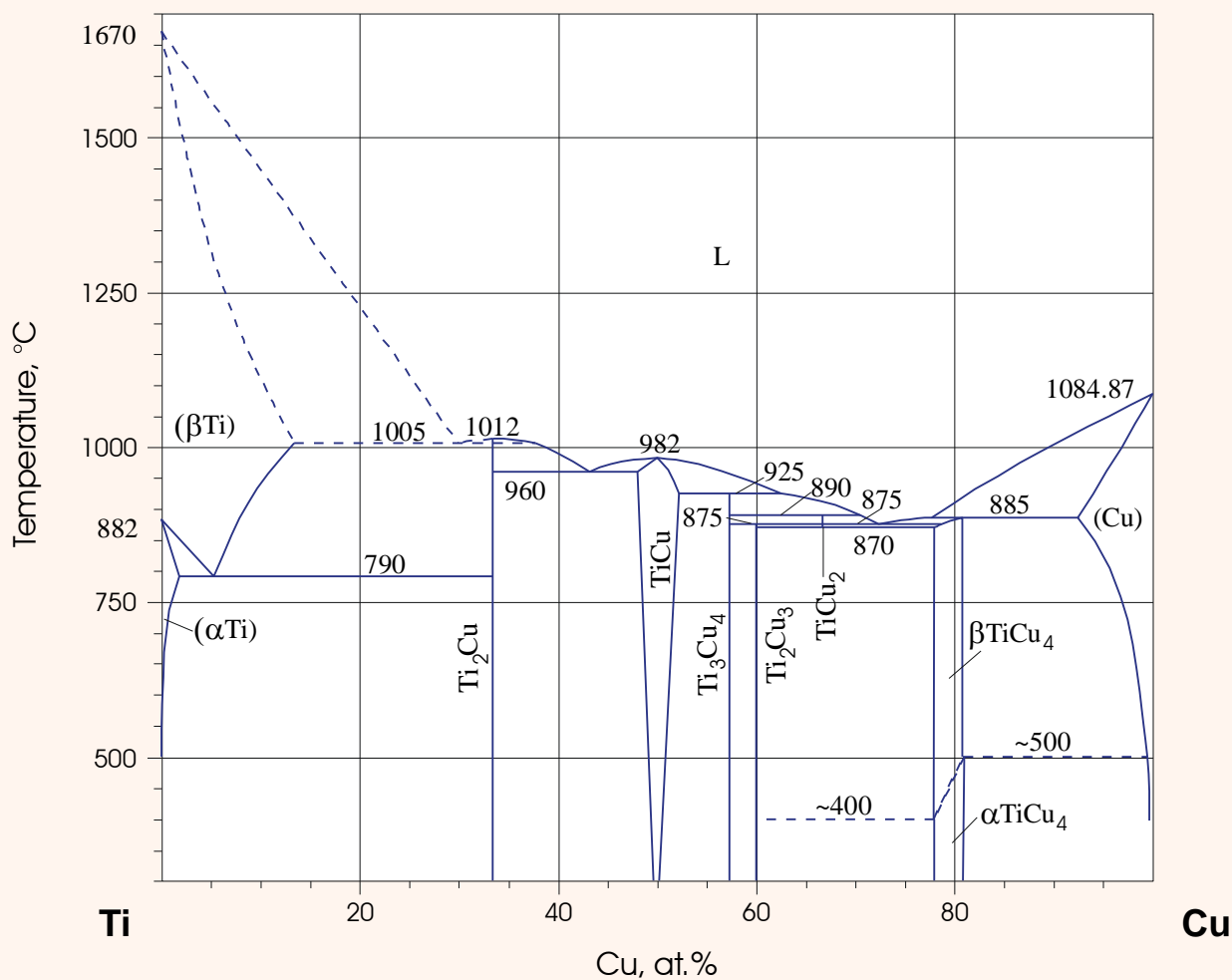
Figure 1: Assessed phase diagram of the Cu-Ti binary system