ASM/NBS NUMERICAL AND GRAPHICAL DATABASE FOR

BINARY ALLOY PHASE DIAGRAMS

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Abstract

Under the ASM/NBS program on alloy phase diagrams, a comprehensive relational database of binary alloy phase diagrams has been developed. The phase diagrams, critical numerical data and crystal structure data of the phases of nearly 1600 binary alloy systems can be accessed by a user friendly database management program. Important features of the database program are: (a) Search and display of all phase diagram graphics prepared for the "Bulletin of Alloy Phase Diagrams" (b) Search and display of the critical numerical data summarizing the "structure" of the phase diagram - the phase reactions, the reaction temperatures, the compositions of the reacting phases, and the crystal structure data of the solid phases.

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The Metallurgical Society, 1988

Introduction

The numerical and graphical database for alloy phase diagrams described herein was developed as part of the ASM/NBS Data Program on Binary Alloy Phase Diagrams. It was felt that the existing phase diagram data literature is so large that a need existed for a computer phase diagram database which would contain the latest binary phase diagrams, all critical points of the diagram, the classified invariant reactions, and the crystal structure data of all solid phases.

The phase diagram database was developed in the Alloy Phase Diagram Data Center, Metallurgy Division in collaboration with the Mathematical Analysis Division of the National Bureau of Standards. The management system for the database is RIM - Relational Information Management System (1). In order to facilitate easy use of the phase diagram database, a user friendly management system designed at NBS called EZRIM has been placed in front of RIM.

At this point, the database contains the binary phase diagrams and the critical data of nearly 1600 binary systems which have appeared in either the Bulletin of Alloy Phase Diagrams (2) or the ASM compendium entitled Binary Alloy Phase Diagrams (3). The crystal structure data and critical equilibria of over 9000 phases are incorporated in the database as well as the reaction temperature and the compositions of the reacting phases of nearly 7300 invariant reactions.

The Data of the Database

The data of a given phase diagram for the database is taken from the computer drawn phase diagram by computer analysis of the labelling of the phase boundaries for the computer graphics program. Preparatory to entering the binary phase diagram into the computer graphics program, the curves of the prototype binary phase diagram plotted on graph paper are labelled according to specific rules associating the phase name with specific phase boundaries. Thus each curve of the phase diagram is entered into the graphics program as a distinct labelled object consisting of digitized data points. The graphics files of these objects are then analyzed by a program called CHALLENGE which performs a geometrical analysis of the diagram to extract metallurgically important features. For example, in the case of an invariant reaction, the program classifies the invariant reactions from the configuration of the six boundary lines that emanate from the reaction horizontal. The program notes the temperature of the reaction and the identity and compositions of the three reacting phases. All of this data is loaded into the database.

The crystal structure data of the phases are loaded using an EZRIM database of space groups, Pearson symbol, prototype and Strukturbericht designations. If the Strukturbericht designation for a phase is known, the other entries are automatically loaded into the database.

The phase diagram database is designated - NUPHAD and is organized according to data pertaining to the alloy system and to individual phases of the system.

For each alloy system, the data filed are:

- o phase diagram graphics and captions
- o diagram type (e.g. simple eutectic)
- o reaction table
  - three-phase equilibria, congruent, critical, tricritical points
  - pure metal transformations
  - phases, compositions, temperature, reaction type
- o phase descriptions
- o publication and update documentation

For each phase, the data files are:

- o crystal structure
  - space group, prototype, Pearson symbol, Strukturbericht designation, comment
- o equilibrium, metastable or high pressure phase
- o stability range
  - homogeneity range and type (e.g. terminal solution, line compound)
  - temperature range and decomposition type (e.g. peritectic, congruent melting, solid state)

The Structure of the Database

The overall structure of the database is given in Figure 1 below. To access the database, one types EZRIM. Since EZRIM works from database files, a prompt for the selection of database file name occurs. NUPHAD is the name of the binary phase diagram database. As shown in Figure 1, NUPHAD is divided into two parts: A SEarch side containing numerical data for data searching and a SHow side which displays the graphical phase diagrams.

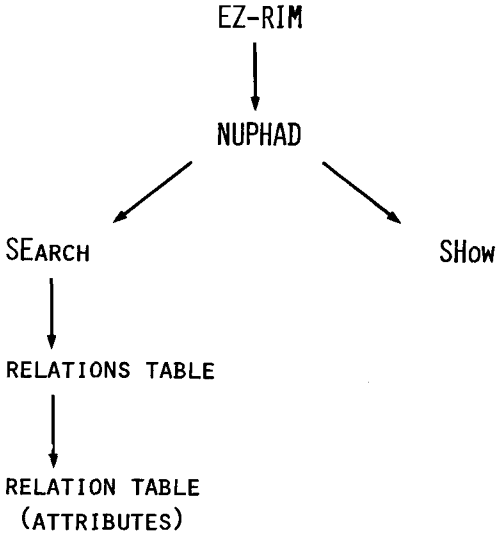

Figure 1. The overall Structure of the Binary Phase Diagram Database.

The SHow side of NUPHAD contains the phase diagrams of approximately 1580 binary systems. If the system has not appeared in the "Bulletin of Alloy Phase Diagrams" (2) its file will contain two diagrams - the weight and atomic percent diagrams that appeared in the ASM compendium "Alloy Binary Phase Diagram" (3). If the system has appeared in the Bulletin, all the graphics prepared for the Bulletin may be displayed - the two basic weight and atomic percent diagrams, diagrams with data points, subset diagrams, metastable diagrams etc.

On typing the command "SH" or "SHow", the following prompt appears:

Alloy System (El-El-El) <MENU> ?

The El in the prompt stands for the element symbol. Enter the element symbol for the two elements of the binary system separated by a dash e.g. Al-Cu. Push carriage return (CR) and a menu of the graphs available for the Al-Cu system will appear. On selection of the specific graphic, the diagram is plotted on the screen or the diagram may be relayed to a printer or plotter.

On leaving the SHow side by typing "Quit", one is moved to the top command position of the database for selection of "SEarch" or "SHow".

Type "SE" of "SEarch" and one enters the Search side of the database. A series of Relations is displayed as shown in Figure 2 below. As noted above, the SEarch side contains all the numerical data of the phase diagrams. These data are arranged in a series of Relations or Tables. The Tables have columns called attributes.

Database: NUPHAD
Number of Relations: 7

	Relation	Attributes	Rows
[01]	BINARY	12	1574
[02]	PHASES	14	9022
[03]	INVARS	15	7298
[04]	CONG	11	3092
[05]	CRITICAL	6	101
[06]	HORDER	15	139
[07]	ELEMENTS	10	103

Figure 2. The RELATIONS TABLE

At the bottom of the Relations table, there is the prompt:

Relation <Binary>?

The desired Relation may be selected from the Relations Table by typing either the name or number of the relation and pushing CR. There is a default in the prompt. Pushing CR without an entry, yields the BINARY relation.

The Relation BINARY contains summary information and publications data on each system in the database. The relations table has 12 attributes or columns and 1574 rows - one row for each system in the database.

Relation: BINARY
Number of Rows: 1574

	Attribute	Type	Length	Description
[01]	ASYST	TEXT	8 CHARS	Alloy system
[02]	PDTYP	TEXT	18 CHARS	Phase diagram type
[03]	NUMPH	INT	8 CHARS	Number of solid phases
[04]	NUMRE	INT	8 CHARS	Number of invariant reactions
[05]	EL[1]	TEXT	2 CHARS	Element symbol #1
[06]	MP[1]	REAL	8 CHARS	Melting point, el. #1 (diagram)
[07]	BP[1]	REAL	8 CHARS	Boiling point, el. #1 (diagram)
[08]	EL[2]	TEXT	2 CHARS	Element symbol #2
[09]	MP[2]	REAL	8 CHARS	Melting point, el. #2 (diagram)
[10]	BP[2]	REAL	8 CHARS	Boiling point, el. #2 (diagram)
[11]	BULL	TEXT	7 CHARS	Bulletin
[12]	UPDATE	TEXT	8 CHARS	Date last revised

Figure 3. The Relation BINARY

PDTYP is a classification according to:

simple [reaction type]	(one invariant reaction)
complex	(more than 1 reaction)
completely mixing	(no reactions)

The BULL entry contains the volume and number of the Bulletin of Alloy Phase Diagrams in which the evaluation was published.

The UPDATE entry contains the date that the information on an alloy system was loaded into NUPHAD.

The Relation PHASES contains detailed information on each phase - crystal structure, homogeneity and stability ranges etc. This relation has 14 columns and there are 9022 rows or phases in the database.

Relation: PHASES
Number of Rows: 9022

	Attribute	Type	Length	Description
[01]	ASYST	TEXT	8 CHARS	Alloy system
[02]	PH	TEXT	24 CHARS	Phase name
[03]	STRKB	TEXT	6 CHARS	Strukturbericht
[04]	PROTO	TEXT	18 CHARS	TPrototype
[05]	PRSON	TEXT	6 CHARS	Pearson symbol
[06]	SG	TEXT	10 CHARS	Space group
[07]	EMP	TEXT	1 CHARS	Condition (equil,meta,P)
[08]	COMNT	TEXT	24 CHARS	Comments on crystal structure
[09]	TY[P]	TEXT	24 CHARS	Phase type
[10]	XMIN	REAL	8 CHARS	Homogeneity range X minimum
[11]	XMAX	REAL	8 CHARS	Homogeneity range X maximum
[12]	UMP	REAL	8 CHARS	Upper melting point
[13]	TMIN	REAL	8 CHARS	Homogeneity range T minimum
[14]	TMAX	REAL	8 CHARS	Homogeneity range T maximum

Figure 4. The Relation PHASES

PHASES contains detailed crystal structure data and also some condensed phase equilibrium information. The main uses of the phase relation are to look up:

- complete structure data for a specified phase or alloy system.
- phases (or systems) with certain structure properties: e.g. of definite structure, space group, or cell type.
- phases of a given stability (homogeneity) range.

The Relation INVARS (the invariant reaction table) has 15 columns. These are 7298 invariant reactions documented in the database. This relation is useful in finding eutectic compositions, maximum solubilities of terminal phases and other phase information related to invariant reactions.

Relation: INVARS
Number of Rows: 7298

	Attribute	Type	Length	Description
[01]	ASYST	TEXT	8 CHARS	Alloy system
[02]	TY[I]	TEXT	16 CHARS	Invariant reaction type
[03]	TP[I]	REAL	8 CHARS	Invariant reaction temperature
[04]	PH[1]	TEXT	24 CHARS	1st phase
[05]	CM[1]	REAL	8 CHARS	Composition of 1st phase
[06]	PH[2]	TEXT	24 CHARS	2nd phase phase
[07]	CM[2]	REAL	8 CHARS	Composition of 2nd phase phase
[08]	PH[3]	TEXT	24 CHARS	3rd phase
[09]	CM[3]	REAL	8 CHARS	Composition of3rd phase
[10]	PROTO[1]	EXT	18 CHARS	1st phase prototype
[11]	PRS[1]	TEXT	6 CHARS	1st phase Pearson symbol
[12]	PROTO[2]	TEXT	18 CHARS	2nd phase phase prototype
[13]	PRS[2]	TEXT	6 CHARS	2nd phase phase Pearson symbol
[14]	PROTO[3]	TEXT	18 CHARS	3rd phase prototype
[15]	PRS[3]	TEXT	6 CHARS	3rd phase Pearson symbol

Figure 5. The Relation INVARS

In TY[1], the invariant reactions are classified by a computer program that analyses the phase diagram graphics. The possible types are:

Eutectic Types	Peritectic Types
eutectic	peritectic
eutectoid	peritectoid
monotectic	syntectic
monotectoid	
catatectic (4)	

When an invariant reaction has the geometry of the Eutectic Types (5) but cannot be definitely assigned to one of the listed eutectic types, it is classified as "eutectic-type". Similarly, invariant reactions with the geometry of the Peritectic Types which cannot be definitely assigned to a listed peritectic type are classified as "peritectic-type".

The Relation CONG shown in Figure 6 below, is a table of congruent points and allotropic transformations set up exactly like INVARS.

Relation: CONG
Number of Rows: 3092

	Attribute	Type	Length	Description
[01]	ASYST	TEXT	8 CHARS	Alloy system
[02]	TY[C]	TEXT	25 CHARS	Congruent type
[03]	MM[C]	TEXT	3 CHARS	Congruent maximum or minimum
[04]	CM[C]	REAL	8 CHARS	Congruent composition
[05]	TP[C]	REAL	8 CHARS	Congruent temperature
[06]	PH[1]	TEXT	24 CHARS	1st phase
[07]	PH[2]	TEXT	24 CHARS	2nd phase
[08]	PROTO[1]	TEXT	18 CHARS	1st phase prototype
[09]	PROTO[2]	TEXT	18 CHARS	2nd phase prototype
[10]	PRS[1]	TEXT	6 CHARS	1st phase Pearson symbol
[11]	PRS[2]	TEXT	6 CHARS	2nd phase Pearson symbol

Figure 6. The Relation CONG

Ty[C] is a classification into:

congruent melting
congruent transformation
allotropic transformation
phase transformation

The Relation CRITICAL is a table of critical points of the miscibility gaps.

Relation: CRITICAL
Number of Rows: 101

	Attribute	Type	Length	Description
[01]	ASYST	TEXT	8 CHARS	Alloy system
[02]	PH[R]	TEXT	24 CHARS	Critical point phase
[03]	CM[R]	REAL	8 CHARS	Critical point composition
[04]	TP[R]	REAL	8 CHARS	Critical point temperature
[05]	PROTO[R]	TEXT	18 CHARS	Critical point prototype
[06]	PRS[R]	TEXT	6 CHARS	Critical point Pearson symbol

Figure 7. The Relation CRITICAL

The Relation HORDER handles higher than first order transitions which may be magnetic or second order.

Relation: HORDER
Number of Rows: 139

	Attribute	Type	Length	Description
[01]	ASYST	TEXT	8 CHARS	Alloy system
[02]	TY[H]	TEXT	10 CHARS	Higher order type
[03]	MM[H]	TEXT	3 CHARS	Higher order max. or min.
[04]	CM[H]	REAL	8 CHARS	Composition of max. or min.
[05]	TP[H]	REAL	8 CHARS	Temperature of max. or min.
[06]	PH[1]	TEXT	24 CHARS	1st phase
[07]	PH[2]	TEXT	24 CHARS	2nd phase
[08]	BC[1]	REAL	8 CHARS	Between composition[1]
[09]	BT[1]	REAL	8 CHARS	Between temperature[1]
[10]	BC[2]	REAL	8 CHARS	Between composition[2]
[11]	BT[2]	REAL	8 CHARS	Between temperature[2]
[12]	PROTO[1]	TEXT	18 CHARS	1st phase prototype
[13]	PRS[1]	TEXT	6 CHARS	1st phase Pearson symbol
[14]	PROTO[2]	TEXT	18 CHARS	2nd phase prototype
[15]	PRS[2]	TEXT	6 CHARS	2nd phase Pearson symbol

Figure 8. The Relation HORDER

The Relation ELEMENTS is a table of selected properties of the pure elements. The melting points listed in this table are the standard ones used for all new diagrams submitted to the ASM/NBS program.

Relation: ELEMENTS
Number of Rows: 103

	Attribute	Type	Length	Description
[01]	NUMBR	INT	8 CHARS	Atomic number
[02]	EL	TEXT	2 CHARS	Element symbol
[03]	NAME	TEXT	13 CHARS	Element name
[04]	MASS	REAL	8 CHARS	Atomic mass
[05]	PMASS	REAL	8 CHARS	Precision (Atomic mass)
[06]	MP	REAL	8 CHARS	Melting point
[07]	PMP	REAL	8 CHARS	Precision (Melting point)
[08]	GROUP	TEXT	5 CHARS	Group in the periodic table
[09]	ROW	TEXT	3 CHARS	Row in the periodic table
[10]	CLASS	TEXT	18 CHARS	Classification (e.g., alkali)

Figure 9. The Relation ELEMENTS

Search Procedures

A relation which contains the objective of the search is selected from the Relations Table (Figure 2). For example, if the eutectics (compositions and temperatures) for various systems are sought, then the INVARS relation would be selected.

At the bottom of the selected Relation table is the prompt:

Select What <ALL>? - the Select prompt.

During the search two other prompts will appear sequentially after the Select prompt:

Sorted By <NONE>? - the Sort prompt.

Conditions <NONE>? - the Search Conditions prompt.

The Select prompt is used for selecting the attributes to be displayed in the output table. The prompt is expecting a list of attributes, and the attributes specified in the list will form the columns in the table which will be displayed. The order of the attributes in the list determines the order of the columns in the table. The <ALL> in the prompt is the default selection. If CR is pushed without an entry, all the attributes will be displayed.

After the selection of the attributes and pushing CR, the Sort prompt will appear:

Sorted by <NONE>?

The Sort prompt allows the output of a search to be sorted prior to being displayed. To specify a sort, enter the attributed by which the output is to be sorted. The <NONE> or default selection means that no sort will be made.

After the selection of an attribute for sort (or none), the final prompt, the Search Conditions, prompt appears:

Conditions <NONE>?

The Search Condition prompt is used to specify the conditions that are being applied to the search. It tells EZRIM exactly what is being searched for. The Syntax of the searching condition is to resemble a FORTRAN IF statement. The general format is:

Attribute name - Boolean operator - value

The Boolean operators and functions are listed in Figure 10.

Operator	Function
eqs	Equals substring (character data only)
nes	Not equal substring (character data only)
eq or =	Equals
ne or <>	Not equals
gt or >	Greater than
ge or >=	Greater than or equal
lt or <	Less than
le or <=	Less than or equal to

Figure 10. Boolean operators

An example of a search condition for Search in the Phases Relation might be:

ASYST eqs Al

This statement sets the condition that the searched for Phases would be from binary Al phase diagrams. Such search condition statements may be stacked separated by an AND/OR connector.

The various strategies of searching cannot be given here but are best learned by operating the database with the user's manual (6) in hand, but some idea of the search procedures and capabilities of the database can be inferred from the sample searches given below.

Sample Searches

In the search shown in Figure 11 below, the INVARS relation was used to search for the eutectic compositions that are between 300 and 600 °C and between 35 and 60% solute. The system, the eutectic composition, and temperature are tabulated. The output was sorted by the binary system (ASYST) attribute.

```
Select what? ASYST,TY[I],TP[I],PH[2],CM[2]
Sorted by?   ASYST
Conditions?  TY[I] EQS eutectic AND
Conditions?  CM[2] GT 35 AND
Conditions?  CM[2] LT 60 AND
Conditions?  TP[I] GT 300 AND
Conditions?  TP[I] LT 500

Search Results -
```

ASYST	TY[I]	TP[I]	PH[2]	CM[2]
Ag-Sb	eutectic	485.	liquid	41.
Al-Mg	eutectic	447.1	liquid	40.151
Al-Mg	eutectic	447.3	liquid	38.725
As-S	eutectic	310	liquid	45.8
Au-Ga	eutectic	448.6	liquid	56.
Au-In	eutectic	455.	liquid	40.5
Au-In	eutectic	495.	liquid	55.3
Au-Sb	eutectic	360.	liquid	35.5
Au-Te	eutectic	447.	liquid	53.
Cd-Sb	eutectic	445.	liquid	57.
Cs-Bi	eutectic	390.	liquid	50.
Cs-Sb	eutectic	459.	liquid	37.964
Cs-Sb	eutectic	404.	liquid	58.396
Cs-Te	eutectic	358.	liquid	55.
K-Bi	eutectic	354.	liquid	50.5
K-Sb	eutectic	460.	liquid	40.582
K-Se	eutectic	360.	liquid	57.
Li-Pb	eutectic	464.	liquid	38.
Li-Sn	eutectic	470.	liquid	43.
Mg-Tl	eutectic	353.	liquid	42.5
Na-Sb	eutectic	435.	liquid	44.438
Na-Sn	eutectic	441.	liquid	38.
Na-Te	eutectic	319.	liquid	57.
Pb-Na	eutectic	333.	liquid	58.86
Pd-Te	eutectic	490.	liquid	35.818
Rb-Bi	eutectic	358.	liquid	50.
Rb-Bi	eutectic	455.	liquid	39.196
Rb-Sb	eutectic	439.	liquid	37.939
Rb-Se	eutectic	355.	liquid	56.118

Figure 11. Eutectic compositions a temperature-composition "box".

Figure 12 shows the output of a search utilizing the PHASES relation for congruently melting phases with upper melting points over 3000 °C. The system, phase type, minimum and maximum homegeneity ranges, and the upper melting points are listed. The search output was sorted by the upper melting point.

```
Select what? ASYST,PH,XMIN,XMAX,UMP
Sorted by?  UMP
Conditions?  TY[P] EQS congruently melting AND
Conditions?  UMP GT 3000

Search Results -
```

ASYST	PH	XMIN	XMAX	UMP
Ti-C	TiC	31.7	48.5	3067.
Ta-B	TaB2	64.143	72.708	3152.08
Hf-Re	HfRe2	62.	67.5	3155.02
B-Zr	B2Zr	32.134	33.475	3213.51
Ti-B	TiB2	65.5	66.667	3223.59
Ti-N	TiN	28.	50.5	3290.
Hf-B	HfB2	64.01	67.653	3370.
Th-O	ThO2	65.	66.7	3390.
Zr-C	gamma	36.373	49.671	3427.
Nb-C	NbC	29.303	50.008	3608.
Ta-C	TaC	36.969	50.368	3825.
Hf-C	HfC	33.713	49.504	3830.

Figure 12. High Melting Phases.

Figure 13 on the next page shows the output of a search utilizing the INVARS relation in which the solubility (> .1% solute) of copper solid solution (Cu) at the intersection with various invariant reactions is shown. The identity and composition of the phase in equilibrium with (Cu) is given. The Al-Cu system was excluded. The search output was sorted by the solubility of (Cu) at the invariant reaction intersection.

```
Select what? ASYST,TY[I],TP[I],PH[1],CM[1],PH[2],CM[2]
Sorted by?   CM[1]
Conditions?  ASYST NES Al AND
Conditions?  PH[1] EQS (Cu) AND
Conditions?  CM[1] GT .1
```

Search Results -

ASYST	TY[I]	TP[I]	PH[1]	CM[1]	PH[2]	CM[2]
Cu-Zr	eutectic	966.	(Cu)	0.105	liquid	6.445
Cu-Hg	peritectic	128.	(Cu)	0.18	Cu7Hg6	46.15
Cu-Tl	monotectic	968.	(Cu)	0.275	liquid	14.5
Cu-B	eutectic	1013.	(Cu)	0.293	liquid	13.3
Cu-Cr	eutectic	1076.6	(Cu)	0.89	liquid	1.56
Cu-Cd	peritectic	549.	(Cu)	2 14	Cu2Cd	33.3
Cu-P	eutectic	714.	(Cu)	3.5	liquid	15.7
Cu-Sb	eutectoid	400.	(Cu)	4.658	gamma	15.361
Cu-Hg	monotectic	660.	(Cu)	5.12	liquid	15.
Cu-Sb	peritectoid	488.	(Cu)	5.712	gamma	15.497
Cu-As	eutectic	685.	(Cu)	5.802	liquid	18.398
Cu-Sb	eutectic	645.	(Cu)	6.06	liquid	18.995
Cu-Sn	eutectoid	350.	(Cu)	6.206	delta	20.529
Cu-As	peritectoid	325.	(Cu)	6.695	beta	12.38
Cu-Sn	peritectic	799.	(Cu)	7.71	beta	13.118
Cu-Sn	eutectoid	586.	(Cu)	9.128	beta	14.868
Cu-Sn	eutectoid	520.	(Cu)	9.128	gamma	16.527
Cu-In	peritectic	710.	(Cu)	10.	beta	18.5
Cu-In	eutectoid	574.	(Cu)	11.	beta	20.15
Cu-Ga	peritectic	916.	(Cu)	16.295	beta	19.976
Cu-Ga	peritectoid	620.	(Cu)	19.976	delta	22.444
Cu-Li	eutectic	180.5	(Cu)	22.6	liquid	99.95
Cu-Zn	peritectic	903.	(Cu)	31.876	beta	36.137

Figure 13. The solubility (> 1% solute) of copper solid solution (Cu) in various systems at the intersection with invariant reactions.

Figure 14 below, shows the output of a search utilizing INVARS in which are listed the Cu-base eutectic systems in which the copper solid solution (Cu) is in equilibrium with a bcc phase. The systems and equilibrium phases are listed.

```
Select what? ASYST,PH[1],PH[3],PROTO[3]
Sorted by?   ASYST
Conditions?  TY[I] EQS eutectic AND
Conditions?  PH[1] EQS (Cu) AND
Conditions?  PROTO[3] EQS W

Search Results -
```

ASYST	PH[1]	PH[3]	PROTO[3]
Al-Cu	(Cu)	beta	W
Cu-Cr	(Cu)	(Cr)	W
Cu-Li	(Cu)	(betaLi)	W
Cu-Nb	(Cu)	(Nb)	W
Cu-Ti	(Cu)	(betaTi)	W

Figure 14. BCC phases in equilibria with (Cu) under eutectic reactions of various systems.

Conclusion

The ASM/NBS Binary Alloy Phase Diagram database is a powerful tool for metallurgical research and alloy development. Besides supplying the most updated version of a given phase diagram, it will give critical phase diagram data needed for alloy design, heat treatment of casting procedures.

It is planned that this database will be made available by ASM INTERNATIONAL initially as an off-line database. The Search side of the database will be put in a form for access by personal computers.

Acknowledgement

The help of Dr. J. L. Murray in the design of EZRIM is gratefully acknowledged. Dr. Murray also wrote the first version of the CHALLENGE program.

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Discussion

V. P. Itkin: Are you planning to include thermodynamic data on your database?

Author's reply: At one time, consideration was given to this. However, it was decided not to incorporate thermodynamic data into the database.

J. R. Rogers: Is there any intention to link the phase diagram database with crystal structure databases?

Author's reply: At present for each phase, the Prototype, the Pearson symbol, the Strukturbericht designation, and the Space Group, if available, are entered in the database either from the phase diagram evaluations published in the Bulletin or from Pearson 3. There are no plans to link the ASM/NBS Phase Diagram Database with any crystal structure databases or any other databases.