Factual Database on Amorphous Materials I*

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Synopsis

Literature and factual database on amorphous materials are being constructed at Institute for Materials Research, Tohoku University. The newly developed KIND integrated materials database system is the base of this project. Numerical and image data are extracted from original manuscripts and stored on the SQL database and on magneto-optical disks, respectively, to realize a multi-media factual database. Several additional programs are written to extract statistical information and utilize this database as a basis of materials design expert system.

I. Introduction

An original literature database on materials has been developed from 1987 at the Institute for Materials Research, Tohoku University (IMR). At present, it contains more than 24,000 literatures on various materials[1]. The most distinguishable feature of this database is that it is an integrated system with relational keyword database on a general purpose machine IBM9370-90 and the digitized images of original papers on magneto-optical disks in HITFILE system. A detailed explanation of the system is given elsewhere[1)] and in the first paper of this volume.

In this materials database we have specifically accumulated information on amorphous materials. This part has a special feature that it contains not only simple keywords but also extracted factual data and the extracted images of phase diagrams and photographs from the original manuscripts. We have discussed and decided necessary items to be extracted from published papers and unpublised information at IMR to construct this factual database on amorphous materials as a really useful one. Especially, concerning the binary alloys we have consulted with the compiled book by Professor Mizutani[2)] and with the amorphous series of the publication RITU[3)].

In section II, the reason of the construction of this database is explained. Section III is for the description of necessary items in the factual database decided by the present research group. In section IV, this newly developed original database on amorphous materials is explained featuring the international offer of this project via academic computer networks. Several examples are introduced

*The 1903th report of Institute for Materials Research in section 5 to indicate the usefulness of this database in practice. Section 6 is devoted to the summary.

II. Demands for Amorphous Materials Database

A number of combinations of important alloys to realize amorphous alloys by rapid quenching method[4] have intensively been studied experimentally at IMR and a number of important findings have already been published.[5-9] Up to the present, the main subjects studied have been binary and ternary alloys. Even only for binary alloys, the number of the data accumulated are very large and it is difficult to remember all of the existing data precisely. Since through the 80's and still at present, amorphous material is one of the most intensively studied subjects at IMR by a number of researchers and the demands for well-managed database on them are very high, the first aim of the present database is decided to be concentrated on the binary alloys.

Very recently, a great progress has been achieved by the discoveries of new amorphous alloy systems. One is the new Al-based ternary amorphous alloys with high strenght and good ductivity[7,8] The other is Fe-Zr-B amorphous system which revealed good soft-magnetic properties after crystallized to nano-scale grains. It is note-worthy that amorphous phase could be formed not only ternary but also even in binary alloys like Al-Ni, Al-Y, Fe-Zr, and Fe-B. This experimental fact implies that amorphous materials with desirable properties could be constructed by the combination of binary systems. If necessary databases on amorphous alloys like the present work have been established earlier, better materials could have been more easily designed by using them.

All the data including experimental conditions are extracted and stored as a factual database under the relational database SQL on the IBM 9370-90 general purpose machine at IMR to meet the demands from the experimental groups at IMR and other researchers widely via national and international computer networks. Especially, a BBS (Bulletin Bourd System) on materials research, MAT-L, on LISTSERV under VM/CMS at IMR is managed by the present research group to serve vivid information on amorphous materials world-widely via Internet (International academic computer network).

III. Extracted Factual Data

According to the demands to this materials databse, it is necessary to extract detailed and correct information from the papers. Necessary items to construct the really useful factual databse on amorphous materials are investigated and discussed for long time with number of researchers at IMR. The present table used for data extraction is shown in Fig.1. There are about 30 items to be extracted including numerical data like Tg and character data like experimental apparatus. Since they are normally not perfectly available, the constructed database is always incomplete.

Actual extraction of the data has been done by several experimentalists on amorphous materials at IMR, and the extracted data are proved (double checked) to be reliable by other researchers.

IV. Constructed Relational Database

At present we have accumulated more than 200 papers as a literature database including the original images of the papers with extracted keywords each up to 4kB according to the standards of KIND. The keywords are open inside Japan to the researchers from the Computer Center of

Amorphous DB Data Sheet(Formation Data/Input data sheet) F 1

Subject	Code	Keyword and Data
1. Reference No.	: 1100	______________ (1 data 1 data sheet) * Reference Data;Author,Reference name,Vol., No,Moth,pp, Etc. include
2. Data No.	: F100	______________ (Reference No + data tag + page) 1) F = Formation data 2) C = Characteristics and numeric data 3) G = Graphic data 4) T = Table data 5) P = Photo,Image data 6) E = Equation data
3. First Category	: F110	1) Formation 2) Thermal Properties 3) Structure 4) Magnetic Properties 5) Electric Properties 6) Superconductivity 7) Mechanical Properties 8) Chemical Properties 9) Etc. (Selection to Category)
4. Second Category	: F120	1) Formation 2) Thermal Properties 3) Structure 4) Magnetic Properties 5) Electric Properties 6) Superconductivity 7) Mechanical Properties 8) Chemical Properties 9) Etc. (Selection to Category)
5. Purposes	: F130	______________ (Less then 10 Word)
6. Classification	: F140 (81)	1) Experiment 2) Theory
7. Chemical Formula of Material	: F150 (91)	______________
8. Name of Material	: F160	______________
9. Output Mark of Phase Diagram	: F162	Yes/No
10. Atomic No.	: F170	______________ (Atomic No.- Atomic No.-Atomic No.)
11. Reference materials	: F180	(Related materials)
12. Preparation Methods	: F190	______________
13. Crucible or Substrate	: F200	______________
14. Processes and Conditions	: F210	______________
15. Outlook of Samples Color,size,shape	: F220	______________
16. Discussion, Conclusion	: F230	______________

Fig.1 Keyword-table to construct the amorphous materials database at IMR.

Tohoku University via campus-wide computer network TAINS connected via N1 network. The computer system at IMR is planned to be open to serve the extracted keywords to the world-wide materials research society via Internet. At the moment, the image information on the magneto-optical disks are only available for the researchers in IMR on their FAX machines set in each laboratory. The copyright fee is automatically applied to the researcher by the system.

An example of the extacted keywords is shown in Fig.2. The first line is for the unique key assigned to the paper. The second line indicates that the image of the original paper is available, if it is Y(yes). Several lines after them are for the title, authors, journal, and keywords (several important ones extracted by ourselves). The last part is for the abstract. These are managed to be stored under the relational database SQL.

```
11 AM920005
21 Y7
31 HASHIMOTO K., NAKA M. and MASUMOTO T.
41 Sci. Rep. RITU, A-Vol. 26 No. 1 (1976) Amorphous Material Issue p. 48-54
51 Effect of Nickel Addition on Corrosion Resistance of Amorphous Iron Base Allo
ys
61 The Research Institute for Iron, Steel and Other Metals
71 Change in the corrosion resistance of amorphous iron base alloys with additio
n of nickel has been studied by electrochemical methods.  The addition of nickel
 to amorphous Fe-P-C alloys increases their corrosion resistance.  In particular
, it improves appreciably the corrosion resistance of the amorphous alloys with
a small amount of chromium.  Nickel added to the chromium-bearing amorphous iron
 alloys does not constitutes a passive film but promotes the formation of a pass
ive film which is mainly composed of hydrated chromium oxyhydroxide.
81 1
91 Fe-P-C, Fe-P-C-Ni, Fe-P-C-Cr
A1 0
B1 0
C1 corrosion resistance, passive film
D1 electrochemical methods
E1 Composition of amorphous iron base alloys, Potentiodynamic polarization curve
s, amorphous FeNiP[13]C[7], Potentiodynamic polarization curves, amorphous FeNiP
[13]C[7] alloys, Potentiodynamic polarization curves, amorphous FeCr[3]NiP[13]C[
7], Potentiodynamic polarization curves, amorphous FeCr[10]NiP[13]C[7], Potentio
static polarization curves, amorphous FeCr[10]P[13]C[7] alloy, Potentiodynamic p
olarization curves, amorphous FeCr[10]Ni[15]P[13] C[7]
```

Fig.2 Sample KIND keywords to construct the literature database.

V. Examples of Usage

In this section, we introduce some of the application programs developed to use the factual and literature database on amorphous materials with sample results.

1. Full-screen retrieval system

One of the most important developing strategy of this database is a convenient human interface. The users of this database is not requested to learn complicated commands to retrieve what they want to search from the database. A complete full-screen interface is given to the users in the present system. The users of this system is requested to remember only the commands to invoke the database; KIND for the general materials literature database and AMOR for the amorphous factual database. After the input of the invoking command, all the necessary inputs are displayed on the screen and most of them are called only pressing a single function key. A sample retrieval screen is shown in Fig.3, which is suitable to select amorphous materials which have necessary properties. All the interface programs are written in REXX and users can change them easily to modify to fit to their usage. The data are stored under SQL database management system. The standard SQL commands are also available to the users who are trained to use the commands directly to achieve better response and more complex retrievals.

```
                                                    AMRPHOUS DATABASE(AMOR)-MAIN
---------------------------------------------------------------------------------
 Material Name  : Al-La

 Category       : formation

 Method         : single roller

 Conditions     :



 Category List  / 1. Formation 2. Thermal 3. Structure 4. Magnetic 5. Electric
                  6. Superconductivity 7. Mechanical 8. Chemical 9. Etc.
---------------------------------------------------------------------------------
 PF1=Help   PF2=Clear     PF3=Quit    PF5=Search
```

Fig.3 Data retrieval screen for the amorphous factual database.

2. Statistical analysis

The research on amorphous materials mainly consists of two groups according to the base-elements; (1) semimetals, like Si or Ge, used for solar batteies, and (2) amorphous alloys, based on metals.

According to the extracted and stored keywords, we have performed fundamental statistical analysis of the data. The first result is shown on the left half in Fig.4 to indicate what kind of elements are studied mostly in the course of research on amorphous materials at IMR. Among 200 papers, just the half of the papers contains the keyword, Fe. The second is Si, the third B, the fourth Ni, the fifth Co, and so on. On the contrary, in the right half in Fig.4 shows the statistics obtained from INSPEC. Among 45,368 papers concerning amorphous materials, 15,877 consern with Si. The second is C. Fe appears as the third. These results clearly show that at IMR, researchers are working mainly amorphous alloys, especially Fe-based alloys. The reason is that Fe-based alloys posess interesting magnetic properties and are expected to be used as magnetic materials in practical applications, which have been the most intensively studied materials at IMR. Easiness of preparation is another important reason should be considered in experimental studies.

The FeB amorphous alloy has been produced to reveal the properties of technological significance for application as soft magnetic materials. Additionally, this alloy is available to be used to investigate crystallization behaviour. The Pd-Si alloy was the first amorphous for the preparation of continuous long ribbons fabricated by Masumoto and Maddin.[4-6]

In Fig.5, we show the most intensively studied alloys stored in KIND and in INSPEC. Fe-B and Pd-Si are the best and the second. The third one is a ternary alloy of Fe-Si-B. In INSPEC, number of papers on binary alloys with Fe is 6,674 and among them Fe-B is the best, which is exactly the same in KIND. For Ni-based amorphous there are 3,999 papers in INSPEC, and 2,966 papers on Al-based amorphous.

No	Element	Present	INSPEC
1	Fe	100	6674
2	Si	69	15877
3	B	68	6499
4	Ni	65	3999
5	Co	46	3406
6	P	40	5928
7	Pd	34	881
8	C	30	11828
9	Cu	29	2013
10	Zr	26	1607

Fig.4 Statistical results on amorphous materials featuring the related elements. The result from KIND is shown on the left and the one from INSPEC on the right.

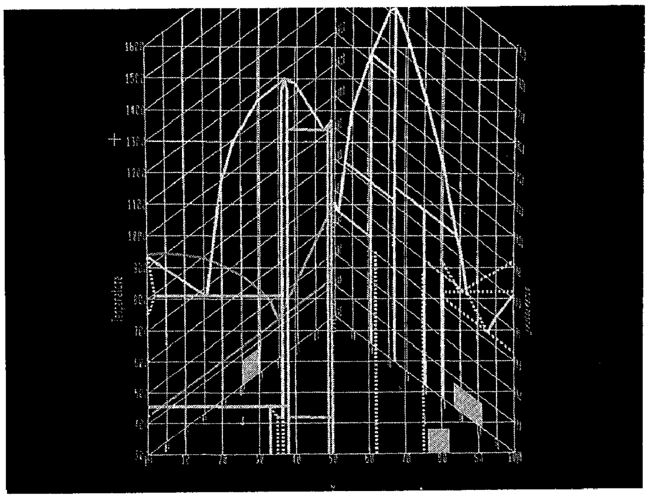
Present		INSPEC					
Fe-B	16	Fe-B	3828	Ni-P	1296	Al-Si	891
Pd-Si	16	Fe-Ni	2124	Ni-Si	1053	Al-Fe	467
Fe-Si-B	12	Fe-Si	2049	Ni-Zr	571	Al-S	325
Cu-Zr	8	Fe-C	1985	Ni-S	483	Al-Cu	271
Fe-Ni-P-B	8	Fe-Co	1626	Ni-Cr	457	Al-Mn	216
Co-Si-B	7	Fe-P	1343	Ni-Al	378		
Fe-P-C	7	Fe-Ge	143				
Fe-P	6	Fe-S	822				
FE-Co-Si-B	5						
Fe-Ni-B	4						

Fig.5 Best alloys studied extracted from KIND and from INSPEC.

Figure 6 indicates the best 10 keywords in KIND amorphous database. The keyword “alloy” is the best, and “structure” the second. These results also support the former consideration that the main research subject on amorphous at IMR is structural material.

STRUCTURE	70
CRYSTALLIZATION	36
GLASS	35
MAGNETIC	28
THERMAL	24
TRANSITION	22
MELT	17
QUENCH	17
LIQUID	16
PHASE	16
STABILITY	16

Fig.6 Top-ranked 10 keywords in KIND amorphous database.



A

La
△
Al Ge

Fig.7 Combined images of three phase diagrams on binary alloys to form a phase diagram for ternary alloy.

3. Image construction -binary to ternary-

Up to the present, we have scanned more than 100 phase diagrams on binary alloys[1] and stored them on the magneto-optical disks. As an example, we show in Fig.7 the combined image of the three phase diagrams on binary alloys to form a phase diagram for the ternary alloy. The figure exhibits an example of stereographically illustrated ternary Al-Ge-La phase diagram which is constructed by three binary system; Al-Ge, Ge-La, and Al-La. The regions indicated by small boxes represent the range of composition for the formation of amorphous phases in the binary systems. In binary system, it has been theoretically and experimentally identified that the amorphous phase is beneficial to be formed at eutectic composition which shows a melting temperature valley. While in ternary system of Al-Ge-La, the range of amorphous phase has been found to be spread over a wide composition range, we believe that it is possible to predict the range of amorphous phase in the ternary system from the combination of binary phase diagrams by taking temperature axes into account. The detailed relation between the re-constructed figure and the real data is being under consideration.

The image of this figure is dynamically moved to see the phase diagram in the three dimension on the dedicated graphics workstation IBM6090. The program was written in PHIGS assuming the IBM6090 graphics capability. This is more desirable to understand the properties of ternary alloys compared to the standard method. Since this image is constructed by a simple combination of three phase diagrams, there is, in fact no information for the ternary alloy at all. It should be studied experimentally and theoretically. It is, however, easier to speculate to fill the middle by using this computer graphics technique.

VI. Summary

Under the relational materials database KIND at IMR, a fuctual database on amorphous materials is being constructed as the first attempt all over the world. Several useful examples have already been tested to use this materials database to extract information among accumulated data.

It is essential to increase the number of data to develop this factual database to open to the international materials research society. We are planning to include most of the existing data on binary and ternary alloys. Especially, high quality unpublished data at IMR will also be included to make this database as the fundamental tool to search for new amorphous alloys with necessary properties by materials design expert system, which is being studied by the present authors.

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