Construction and Application of Materials Database for Non-Equilibrium and Metastable Phases[†]

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The Institute for Materials Research, Tohoku University (IMR) is a collaborative research institute and open to scientists all over the world. Research subjects of IMR covers most advanced materials of non-equilibrium and/or metastable phases. In order to contribute an original materials database on these research subjects, a comprehensive project was started in 1987. As a result of 11 years of continuous effort, an integrated database system consisting of both literature and numerical factual databases has been constructed and become one of the largest systems in Japanese universities. This paper introduces the details of the management systems, utilization interfaces and contents of the database system, as well as the future IMR database projects.

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I. Introduction

In the early years of the Institute for Materials Research (IMR), Tohoku University, when it was called the Research Institute for Iron, Steel and Other Metals, the researchers worked mainly on the crystalline phases of metallic alloy systems. In order to meet the present-day high technology demands, the modern research areas of IMR have been expanded to cover most of the advanced materials, which are thermodynamically non-equilibrium and/or metastable phases, such as amorphous metallic materials, nanoscale materials, magnetic metallic multilayers (superlattices), functionally gradient materials, ultrahigh pressure and/or temperature materials, as well as high T_c superconducting materials and biomaterials.

Since 1987, when IMR was reorganized as a collaborative research institute, which is open not only to Japanese but also to foreign scientists, the research work has become even more extensive and rapid progress has been and is being made. As a result, more than 500 scientific papers in English are published annually. In order to contribute an original materials database on the variety of research subjects at IMR, a computerized materials database project KIND was also initiated in 1987 as an institute-wide activity which is open to the world via computer network. On the basis of KIND, two factual database projects, AMOR and MAGNE were started in 1993 and 1996, respectively.

This paper introduces KIND, AMOR and MAGNE database systems. Details of their management systems,

utilization interfaces and contents are described. The final summary ends with a brief description of future IMR database projects.

II. KIND: A Materials Database System

The computerized materials database KIND (KINken Materials Database, derived from the Japanese name of the Institute) was started in 1987 to contribute an original materials database on the variety of research subjects mentioned in the previous section. KIND is an integrated database system, consisting of both a literature database and several numerical factual databases.

Primarily intended to be a collection of papers published by IMR members, KIND soon was expanded to include papers published all over the world which treat topics in IMR's fields of interest. More than 6500 papers are handled annually and the literature data now totals more than 70000 pieces, making it the largest literature database ever created by a Japanese university.

All the collected copies of papers are checked by specialists or experts in the relevant field. The literature data extracted from an original paper consists of 14 items, including KIND serial number, author(s), journal, page number, title, affiliation(s), abstract, classification (experimental/theoretical), materials (combination of constituent elements), structure(s), preparation method(s), physical and chemical properties, measurement method(s) and captions of figure(s) and/or table(s). The total amount of information for each data is at most 4KBytes. These data are rearranged to form SQL database with several connection schemes. The figures, tables, graphs, and photographs in the papers are separately stored on the CD-ROM and can also be accessed. The whole database system is managed under a

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VM/CMS operating system on an IBM mainframe computer ES9000/9121 at IMR.

It should be noted once again that more than 6500 original papers are treated annually for the construction of KIND. Handling such a large volume of literature is of course very costly in terms of both time and money, especially when this is all done manually. In order to reduce costs, a support system was developed in KIND consisting of six interface programs. Two of these programs were written in BASIC language; one for checking mistakes in the input data and listing them in a format which could easily be corrected, while the other converts the input data into a suitable form for submission to different host machines. The remaining four programs were written in REXX language. The first is for automatic index data making, submitting and management; the second for automatic dictionary type data making, submitting and management; and the remaining programs for searching data and statistical analysis.

User-friendly and highly efficient utilization systems have been developed and implemented so that the users can make full use of KIND without any difficulty. To retrieve KIND, for example, one simply enters the command "KIND" on VM/CMS. Searches then proceed by means of a full-screen user interface. The user need only select necessary items or input keywords. The necessary keywords are constructed by combining them with "and (&)", "or (|)", and "not (—)". After retrieval, KIND informs you of the number of papers which have matched the request. If the number is too large to see, it can be reduced by reusing the same screen with additional keywords. Information can be obtained on (i) title, (ii) author(s), (iii) journal, (iv) keywords, (v) abstract, and so on. More information could be obtained if KIND is retrieved using SQL commands directly.

KIND can be accessed from anywhere in the world via Internet. Users can, as a matter of fact, access KIND in three ways: World Wide Web (WWW), tn3270 and telnet (vt100), which can be easily found on IMR's WWW home page (<http://www.imr.tohoku.ac.jp/index.html>).

The first screen of KIND on WWW shows the following five items: (1) Basic KIND Database; (2) KINLIB (IMR) Database; (3) Dictionary KIND Database; (4) KCHART (Chart of IMR); and (5) AMCHART (Chart of AMORPHOUS).

(1) is the basic database of KIND. (3) is the same basic database as (1), but is arranged in dictionary-style. (1) and (3) both give access to the Library Retrieval System where there are five subdatabases, *i.e.* *Kinlib*, *Csuper*, *Imc*, *Amorphous* and *Cluster*.

Kinlib deals with papers published by IMR researchers. *Csuper* is a literature database for high T_c superconducting materials. *Imc* is a short form of Intermetallic Compound and contains literature data for magnetic intermetallic compounds, as well as for other magnetic materials, particularly magnetic metallic multilayers (superlattices) and ultrathin films. *Amorphous* gives literature data for almost all the

metallic materials of non-equilibrium phases. It should be noted that *Amorphous* should not be confused with AMOR database, a numerical factual database described in the next section. The last one, *Cluster*, is a literature database for granular microcluster or nanoscale materials.

(2) is a literature database extracted from IMR published papers, containing the following items: Total Number of IMR Papers, Papers with Specified Element(s), Papers with Specified Keyword(s), Papers by Research Group(s). (4) is a representation of (2) in chart form, allowing one to see at a glance the change of main subjects on an annual basis and the research development at IMR.

(5) is the numerical factual database for amorphous alloys which is described in the following section.

III. AMOR: A Factual Database

In 1993, the factual database project AMOR was started. As is clearly seen from the name AMOR, which are the first four characters of "amorphous". This project aimed at extracting and utilizing numerical data of formation ability and physical properties of metallic amorphous alloys. Special attention was initially paid to ternary amorphous alloys. At present, however, not only the alloys of pure amorphous phase, but also those of other non-equilibrium phases such as quasicrystalline, microcrystalline, etc., are included in AMOR.

To date, 8327 points of formation data of 1532 ternary amorphous alloys, consisting of 351 ternary systems have been extracted, classified and evaluated. In order to gather all these data, a systematic publication survey was conducted, including both internal reports and regular journals worldwide. As a result, quite a large number of previously unpublished formation data of ternary amorphous alloy systems of great industrial importance were discovered and adopted. To the best knowledge of the authors, all the experimentally observed formation data of ternary amorphous alloys reported in the publications surveyed have now been comprehensively collected.

A detailed data distribution survey revealed that contributors are distributed among 370 research institutions in 34 countries and regions. It also revealed that Japan's contributions are the highest (45% of the published papers and 52% of the number of alloys systems). The USA and Germany come next, followed by the UK and China. It should be noted that IMR published 326 papers concerning with 609 ternary amorphous alloy system, representing about 75% contributions in Japan and 40% worldwide.

From the above, it is evident that IMR should take charge of constructing factual database for amorphous alloys, which is really the only one in the world to date.

The original formation data of all possible phases for each ternary alloy system containing amorphous phase are presented in both triangle phase diagrams and tables of numerical data. The phases are classified into (i) amorphous, (ii) amorphous plus crystalline, (iii) crystal-

line, (iv) quasicrystalline and (v) others which are marked in the phase diagrams by black circle, half black half white circle, white circle, black triangle and black square, respectively, while in the numerical tables by short form of AM, AC, CR, QC and OT, respectively.

In addition to the formation data themselves, the experimental conditions, sample form and size, phase identification methods to each point of formation data, and comment on the amorphous alloy system are listed above the numerical tables. The list order is (1) preparation method of master alloy, (2) preparation method of amorphous alloy, (3) atmosphere for preparation of amorphous alloy, (4) sample form and size, and (5) phase identification method followed by reference and comment.

Preparation methods of master alloys include (i) radio frequency melting, (ii) arc melting, (iii) resistancy-heat melting, (iv) levitation melting, (v) electron beam melting, (vi) laser beam melting, and (vii) plasma melting. Among these methods, radio frequency melting and arc melting are the most widely used.

Preparation methods for amorphous alloys are of prime importance in the experimental conditions which provide the basis for the classification of amorphous alloy systems. Unlike that for master alloys, there are a great number of methods, from the technological viewpoint, for preparing the final amorphous alloys. However, the variety of methods can be classified into three main groups from the physicochemical principles, that is, solid reaction (from solid to solid), liquid condensation (from liquid to solid) and gas condensation (from gas-atomic vapor-to solid).

The following methods can be found in the solid reaction group: (i) mechanical alloying, (ii) hydrogen absorption, (iii) irradiation, and (iv) chemical reduction (coating). Although these four methods belong to the same group, they are usually applied to some special alloy systems different from each other. Even they are applied to the same alloy system, the formation data of amorphous alloys are quite different.

In the liquid condensation group, there are (i) melt-spinning, including single or twin roller spinning and in-rotating water spinning, (ii) water quenching, (iii) gas atomization, (iv) chill-casting, including metallic mold casting, (v) piston-anvil method (splat cooling), and (vi) other liquid quenching methods. Different methods in this group are applied to obtain different shapes and sizes of the desired amorphous alloys and for the same alloy system the formation data of amorphous phase are usually not of significant difference.

The gas condensation group includes (i) sputtering and (ii) vapor deposition methods. When applied to the same alloy system, the formation ability of amorphous phase by these two gas condensation methods is usually bigger than that by liquid condensation. For some alloy systems, it is impossible to realize amorphous phase by liquid condensation, but possible by gas condensation. From the above, it is clear that the formation data of amorphous phase depend upon the preparation methods,

and that the data obtained by different methods should not be merged in principle. For the formation data of other non-equilibrium phases, the situation is similar to that of the amorphous phase.

It should be noted that most of the amorphous alloys are prepared by liquid condensation method, in particular the melt-spinning method.

The atmosphere usually includes argon gas, helium gas, hydrogen gas, nitrogen gas, air, vacuum and so on. A sample form of amorphous alloy is usually ribbon-shaped, wire, rod, foil, thin film and etc., and the sample made by mechanical alloying is usually bulk amorphous alloy. Very few are in powder forms. As for the phase identification methods, there are various kinds of methods which can not be listed due to the limit of pages. Nevertheless, the most widely used methods are X-ray diffraction (XRD), transmission electron microscopy (TEM), and scanning electronic microscopy (SEM).

It should be pointed out that part of the above information, that is, formation data of the 351 ternary amorphous alloy systems is available in AMOR, but the complete information can be found in *Non-equilibrium Phase Diagrams of Ternary Amorphous Alloys*, sub-volume A of volume 37, Landolt-Börnstein New Series, edited by Yoshiyuki KAWAZOE, Jing-Zhi YU, An-Pang TSAI and Tsuyoshi MASUMOTO, published by Springer-Verlag in 1997.

As the collection of formation data of the above 351 ternary amorphous alloy systems is completed, the next to do is to extract, classify and evaluate numerical data of mechanical, physical, chemical and other important properties, which will be presented partially in AMOR, but completely in subvolume B of the databook series mentioned above. Therefore, the two subvolumes provide complete information concerning with ternary amorphous alloys.

Together with the treatment of the data of ternary amorphous alloys, the data for multicomponent, *i.e.* quaternary, quinary, . . . metallic amorphous materials are also under preparation, as they are even more important from the viewpoint of industrial applications. The data of these multicomponent systems will be presented in both AMOR and subvolume C.

Crystallization of the amorphous phase is a good way to obtain new metallic materials with very special phases, for instance, materials with micro- or nano-crystals dispersed in the amorphous matrix; materials consisting of pure micro- or nano-crystals; materials of quasicrystals, and so on. These materials are very important for industrial applications and/or basic research in physics.

The data of all these materials made from amorphous alloys by a crystallization process are being extracted, classified and evaluated and will appear in both AMOR and subvolume D.

IV. MAGNE: A Factual Database

Another factual database MAGNE was started in 1996, with the aim of extracting and utilizing numerical

data for magnetic metallic multilayers (superlattices).

As mentioned in the previous sections, magnetic metallic multilayers (superlattices) is also one of the modern research areas at IMR. A large amount of literature information concerning with magnetic metallic multilayers has been collected and stored in KIND, among which there are more than 6000 papers containing numerical data which are important to both basic and application researches. At present, the numerical data for about 200 binary multilayer systems are being extracted. The data extraction for multicomponent systems will be started after the completion of the binary ones.

Data in MAGNE for each multilayer system are divided into three groups: (1) properties, (2) experimental measurement method(s), and (3) theory and simulation(s). Data in group (1) and (3) are presented in forms of graph(s), numerical table(s), equation(s) (formula) and/or parameter(s). While data of group (2), *i.e.* description(s) or statement(s) of experimental measurement method(s) are listed below caption(s) of graphs and/or numerical tables, followed by comment(s).

As for the items in the above data groups, properties group includes: (1) interlayer exchange coupling (indirect anti-ferromagnetic interlayer exchange coupling, oscillatory behavior of interlayer exchange coupling with interlayer thickness, RKKY-type interaction, 90° coupling or non-Heisenberg-type coupling, quantum well structures, artificial long-period magnetic structures (antiferro-, ferri-, and helical-magnetism, etc.), exchange spring magnets); (2) giant magneto-resistance (MR) (spin-dependent scattering of conduction electrons, interface roughness, coupled and non-coupled multilayers, spin valves, current-in plane MR (CIP-MR), current-at-an-angle-to plane MR (CAP-MR), current-perpendicular-to plane (CPP-MR), mean free path and spin diffusion length); (3) perpendicular magnetic anisotropy (interface magnetic anisotropy and magneto-elastic anisotropy); (4) magneto-optical effect (enhancement of Kerr effect at the plasma absorption edge, magnetic polarization at interfaces, magneto-optical recording media and quantum size effect); (5) interface magnetism (enhancement of magnetic moments and two-dimensional magnetism); (6) soft magnetic properties (permeability, coercivity, hysteresis curves and saturation magnetic flux density).

The following items can be found in the experimental measurement method(s) group: (1) sample's preparation (sputtering, UHV deposition and electro-deposition), (2) measurements of magnetization and magnetic anisotropy (vibrating sample magnetometer (VSM), superconducting quantum interference device (SQUID), magneto-optical Kerr effect (MOKE), Torque-meter, ferromagnetic resonance (FMR)), transport (CIP-MR, CAP-MR, CPP-MR, Hall effect, magneto-thermal conductivity,

magneto-thermopower), MOKE spectra (Kerr rotation θ_K and ellipticity η_K), surface magneto-optic Kerr effect (SMOKE)), light scattering technique (Brillouin scattering and Raman scattering), spin polarized technique (spin-polarized low-energy electron diffraction (SPLEED), spin-polarized electron energy loss spectroscopy (SPEELS), scanning electron microscopy polarization analysis (SEMPA)), polarized neutron diffraction, nuclear magnetic resonance (NMR), Mössbauer spectroscopy (conventional ^{57}Fe Mössbauer spectroscopy and conversion electron Mössbauer spectroscopy (CEMS)), Muon spin rotation, relaxation and resonance (μSR), and microscopy (MOKE microscopy, Lorenz electron microscopy, magnetic force microscopy (MFM)).

In the theory and simulation(s) group, there are: theoretical analysis and/or computational simulation results on electronic structure, spin structure, phase transition, Kerr effect, interface magnetism and so on.

It should be noted that the complete information for the magnetic metallic multilayers would also be published by Springer-Verlag as a new volume of Landolt-Börnstein series.

V. Conclusions and Future Projects

The integrated materials database KIND and its offshoots, the factual databases AMOR and MAGNE constructed at IMR have been introduced. It should be noted that KIND is publicly accessible by computer network, while AMOR and MAGNE are not for the time being. Of course, these two factual databases will be also open to the world through internet after their completion in the near future.

The next data projects will be a factual database for ultrahigh pressure and/or temperature materials, and a factual database for nanoscale materials. There are special research groups at IMR working exclusively on ultrahigh pressure and/or temperature materials and nanoscale materials, with both the experimental and the first principles computer simulation methods. Several hundred papers have already been published and accumulated in KIND.

The final aim of IMR data projects is to offer fundamental information on highly selected materials for industrial use.

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