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Review

Factual Databases for Materials Design and Manufacturing

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The present status of scientific and technological factual databases is reviewed. The number of source information which should be entered into a materials database is very large, therefore the databases must be optimally structured in records and files As an example, the structure of JICST TH (the Japan Information Center of Science and Technology Thermophysical and Thermochemical Property Database) is presented. Discussion is made on characteristics of data items, validation of materials databases, the present status and future aspect of delivery and database systems.

KEY WORDS: materials database; factual database; database building; architecture; database system; delivery system; on-line search.

1. Present Status of Scientific and Technological Factual Database Building

Well known bibliographic databases such CA (Chemical Abstracts) Search, MEDLARS (MEDical Literature Analysis and Retrieval System) and INSPEC (INformation Service in Physics, Electrotechnology and Control) are designated as ' reference database ', because they provide orientations to the source documents. On the other hand, factual databases allow us to access directly to the source information that represents ' fact '.

Among some attempts[1] for classification of the types of databases, it seems very relevant at present to use the classification by Cuadra,[2] as shown in Fig. 1. The available scientific and technological factual databases amount nearly three hundred in the world.[3-7] They can be classified into numeric, numeric-textual, full-text, graphic or image, and sound according to their data form. About a half of the databases can supply numerical data through on-line access.

For development of new materials, various data are necessary for material design. Accompanied by the extension of needs and importance of materials information systems, a variety of materials databases have been constructed as factual databases for material design and manufacturing.[8-15]

Representative materials databases are summarized in Table 1.[16] Material types covered by these materials databases are metals, refractories, superalloys, ceramics, glasses, composites, inorganic and organic compounds, plastics, semiconductors, woods, and others. These databases provide the information on materials properties such as mechanical properties, chemical properties, thermal, electrical–electronic, and other physical properties, corrosion–oxidation, and processability.

Table 2 shows detailed information of these databases such as the contents of data, producer, distribution system and full name of each database.

Since each materials database has a complicated data structure and specific search functions, construction of a database needs much money and manpower and expertise of skilled researchers. Therefore many of these databases are constructed by governmental organizations or national research institutes, sometimes by their cooperation, in financial support of national funds.[17]

In addition, a great deal of effort is necessary for compilation and evaluation of different types and levels of data which are diversified widely. Therefore it has been recognized that interlinking of databases in various organizations, international cooperation and standardization are very important for establishing and distributing databases.[18,19] In fact, many projects started through the conferences: " Workshop on Computerized Materials Data Systems " at Fairfield Glade, Tennessee, USA in 1982.[20] " CEC Workshop on Material Data Banks " in 1984 at JRC (Joint Research Center) Petten,[21] CODATA (COmmittee on DATA for science and technology) International Conferences, (9th (1984) at Jerusa-

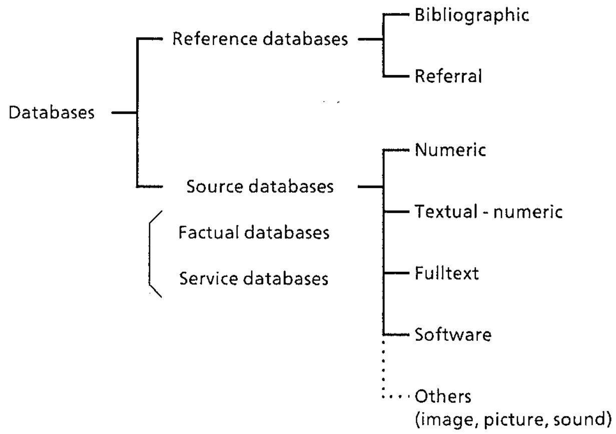


Fig. 1. A classification of databases suggested in a directory of on-line databases.[2]

Table 1. Representative materials databases.

Properties	Materials				
	Chemical substances	Metals and Alloys	Plastics and Woods	Semiconductors and Ceramics	Others
Chemical properties	CAS ONLINE, RNSS, SANSS, MERCK INDEX, JICST DC	CORROSION	(CORROSION)	(CORROSION)	
Physical properties	DIPPR, F*A*C*T*, JANAF, ICSD, CSD, THERMO, JICST TH*	THERMO-CALC, THERDAS, STEEL-FACTS, CRYSTMET, (MDF/1)	POLY-PROBE, (DETER)	EMIS, DETER,	---
Mechanical properties	---	MDF/1, ZLC, BOLTS, CDC, DTDATA, PVS, CUTDATA	ERIS	---	---
Spectra	MSSS, WMSSS CNMR, ID-IR, IRSS, SDBS	---	---	---	---
Others	RTECS, DATA-BANK, GENETYX, THE PRESTICIDE	CASIS, MATERIALS SELECTOR, CAPRICORNIA	POLYMAT, (ERIS)	---	EMBL-GDB, GENBANK, NBRF-PDB, PRF-SEQDB

( ) represents repeated appearance.

lem,[22] 10th (1986) at Ottawa,[23,24] and 11th (1988) at Karlsruhe[25]) and " CODATA work shop on Materials Data Systems for Engineering " in 1985 at Schluchsee.[26]

In the USA, NIST (National Institute of Standards and Technology), formerly NBS (National Bureau of Standards), and DOE (Department of Energy) started a cooperating project of MIST (Materials Information for Science and Technology) in 1983 for the purpose of evaluating of a computer network of materials databases using a gateway system.[27] Based upon this technology, National Materials Property Data Network, Inc. was established, and an experimental MPD (Materials Property Data) network is now in operation.[28,29] Committee ASTM E-49 is devoted to the standardization of databases.[30-32]

In Europe, CEC (the Commission of the European Communities) JRC at Petten and Ispra began to build the HTM-DB (High Temperature Materials Databank).[33] Similar projects are under way in several countries in EC.[34] To interconnect these European hosts, CEC developed a European Host Network (EHN) in a five-year " Program for the Development of the Specialized Information Market in Europe " (1984–88). One of the priority area of the program is factual materials data banks. The Materials Data Banks Demonstrator program is also on progress.

In Japan, some organizations take part in several international cooperative projects.[35] STN (the Scientific and Technical Information Network) International is operated by three database producers of JICST (the Japan Information Center of Science and Technology), CAS (Chemical Abstracts Service) in the USA and FIZ (Fach Informations Zentrum) Karlsruhe in the Federal Republic of Germany,[36] and links each center through international dedicated telecommunication lines. Searchers can access any of the databases stored at the service centers, using a common command language, through the nearest STN service center. In ' Versailles Project for Advanced Materials and Standards ' (VAMAS) agreed on at Versailles Summit in 1982, Japanese organizations are also actively participating.[37] In Technical Working Area " Materials Data Banks ", JICST, National Research Institute for Metals (NRIM), Governmental Research Institute, Nagoya (GRIN) and National Chemical Laboratory for Industry (NCLI) are conducting joint research.

2. Design of Materials Databases

Original source data for inclusion in materials databases have many items, and they often are represented in complicated data structure such as vector, hierarchy or network. In construction of a database, these source data items are structured to a record which is the information unit of a datafile. Data structure of the record is designed to conform with the purpose of their use, for instance on-line search or data transfer in tapes.

2.1. Data Items and Structuring of Records and Files

Typical data items of materials databases are presented in Table 3. Each data item is correlated with the other items, so it is necessary to select an appropriate database structure among simple linear structure, multi dimensional relational structure, and net-

Table 2. Profiles of representative databases.

Field	Database	Contents	Producer (Nation)	Delivery system and network
Chemistry	JICST DC	Chemical dictionary	JICST (Japan)	JOIS-F
	CAS ONLINE	Chemical dictionary	Chemical Abstracts Service (USA)	STN International
	RNSS[1]	Chemical Abstracts registry file	Chemical Abstracts Service (USA)	STN, DIALOG, Questel, ORBIT
	SANSS[2]	Chemical dictionary	Chemical Information Systems (CIS) (USA)	CIS
	MERCK INDEX	Merck Index	Merck & CO., Inc.(USA)	CIS, BRS
	HELIBRON	Organic and organometallic compounds	Chapman and Hall Ltd. (UK)	DIALOG
Physics	JICST TH*	Thermo-physical and chemical properties	JICST (Japan)	JOIS-F
	JANAF[3]	Thermo-physical and chemical properties	National Institute of Standards and Technology (NIST) (USA)	STN International
	ICSD[4]	Crystal structure of inorganic substances	Institute of Inorganic Chemistry, Bonn University (FRG)	STN International, CISTI
	CSD[5]	Crystal structure of organic substances	Cambridge Crystallographic Data Center (UK)	CISTI
	THERMO[6]	Thermodynamic properties	NIST - Texas University (USA)	CIS, STN International
	DIPPR[7]	Physical properties	American Institute of Chemical Engineers (USA)	STN International
Spectra	JICST MS	Mass spectra	JICST (Japan)	JOIS-F
	IRSS[8]	Infrared spectra	U.S. Environmental Protection Agency (EPA) (USA)	CIS
	CNMR[9]	Carbon-13 nuclear magnetic resonance spectra	Netherlans Information Combine (Netherlands)	INKADAT
	ID-IR	Infrared spectra	Asahi Research Center (Japan)	MARK-III
	MSSS[10]	Mass spectra	NIST-EPA-NIH(National Institutes of Health) (USA)	CIS
	SDBS[11]	Spectra of IR, Mass, H-NMR, and C-NMR	National Chemical Laboratory for Industry (Japan)	Direct dial
Engineering	CORROSION	Corrosion of metals, alloys, carbons, plastics and glasses	Marcel Dekker, Inc. (USA)	ORBIT
	EMIS[12]	Properties of Si, GaAs, InP, and $LiNbO_3$	Institution of Electrical Engineers-INSPEC (UK)	BRS
	DETER[13]	Deterioration of metals, plastics, and organic compounds	Plastics Technical Evaluation Center (USA)	Magnetic tape release
	DETHERM[14]	Chemical engineering data	DECHEMA (FRG)	INKADAT
	POLYPROBE	Physical, mechanical, thermal and electrical properties of plastics	International Plastics Selector, Inc. (USA)	Tymnet, Telenet
	MDF/ I [15]	Mechanical and physical properties of iron and nonferrous metals	ASM International (USA)	ORBIT
	ZLC[16]	Mechanical properties of zinc, lead, cadmium and their alloys	Zinc Development Association (UK)	DATAPAC, DATEX-P, Euronet
	BOLTS[17]	Mechanical and thermal properties of bolt materials	Materials Research and Computer Simulation Co.(USA)	Direct dial
	CDC[18]	Physical, mechanical, electrical and corrosive properties of copper	Copper Development Association, Inc. (USA)	Battelle Columbus
	DTDATA[19]	Damage, cracking, and tolerance data of steels and nonferrous alloys	University of Dayton, Research Institute (USA)	Magnetic tape release
	CUTDATA	Machinability of steels, nonferrous alloys and nonmetals	Metcut Research Association, Inc. (USA)	Magnetic tape release
	STEELFACTS/T[20]	Properties of iron and steel	Betriebsforschungs-Institut (FRG)	DATEX-P
	CAPRICORNIA	Properties of steels, nonferrous alloys, and plastics	Capricornia Institute of Advanced Education (Australia)	Magnetic tape release
	POLYMAT[21]	Catalog of commercial plastics	Deutsches Kunststoff Institut (FRG)	INKADAT

1) Registry Nomenclature and Structure Service.
2) Substructure And Nomenclature Search System.
3) JANAF thermochemical table.
4) Inorganic Crystal Structure Database.
5) Cambridge Structural Database.
6) Thermodynamics.
7) Design Institute for Physical Property Data.
8) Infrared Search System.
9) Carbon-13 Nuclear Magnetic Resonance Search System.
10) Mass Spectral Search System.
11) Spectral Data Bank System.
12) Electronic Materials Information Service.
13) Materials Deterioration Data Program.
14) DECHEMA Thermophysical Property Data Bank.
15) Materials Data File I.
16) Zinc, Lead, and Cadmium.
17) Bolting Database.
18) Copper Data Center.
19) Damage Tolerance Database System.
20) Materials database: Steel and Iron / Test values.
21) DKI Polymer Materials Properties Database.

Table 3. Main data items of data in materials databases.

	Materials			
	Chemical substances	Metals and Alloys	Plastics and Woods	Semiconductors and Ceramics
Material identifier	Compound code, Common name, Chemical name, Molecular formula, Composition	Material type, Code (ASTM, AISI, JIS), Common name, Composition	Common name, Formula, Composition, Commercial name, Species	Common name, Composition, Producer
Property data	Molecular structure, Physical property, Spectra	Mechanical property, Corrosion data, Machinability, Physical property, Processsability, Phase diagram	Physical property, Mechanical property, Thermal property, Electrical property, Processability	Electrical property, Processability, Strength, Mechanical property
Auxiliary information	Compound class, Synthesis, Sample, Measurement condition	Heat attribute, History, Testing condition, Sample form, Welding, Sampling location	Primer, Mixing ratio, Producer, Processing, Testing condition, Sampling, Comments	Processing, Measuring method, Phase diagram, Photographs
Reference information	Journal: name; issue (volume, number), Publication year, Author, Organization, Title of document	Journal: name; issue (volume, number), Publication year, Author, Organization, Title of document	Journal: name; issue (volume, number), Publication year, Author, Organization, Title of document	Journal: name; issue (volume, number), Publication year, Author, Organization, Title of document

work structure.

Spectrum databases (MSSS, IRSS, *etc.*) and chemical substance databases (CAS ONLINE, RNSS, *etc.*) presented in Table 1 have relatively simple data structures, but databases for physical properties (DIPPR, FACT, *etc.*) and mechanical properties (MDF/1, ZLC, *etc.*) have complex data structures corresponding to the relations within each data items.

As an example for deeper understanding on data items and structuring of records to data files, JICST TH (Thermophysical and Thermochemical Property Database, indicated by * in Tables 1 and 2) will be presented.[38,39]

The outline of data items of JICST TH is shown in Table 4. Material identifiers are chemical name, common name, molecular formula, element species, molecular weight, substance code and so on. The data items of property data are numerical values of sixty types of material properties (*e.g.*, density, sound velocity) with their units and variables in measurement (temperature and pressure). The data items qualifying the values such as the physical state and error in measurement may be added. In addition, thirteen data items concerned with reference information are included.

Since over one hundred data items of JICST TH have a complex hierarchy structure, the data file is divided into three subfiles in order to simplify and shorten the record format. The outline of record and file structure in the search system are presented in Fig. 2.[38] One of three subfiles is a substance file (S file) which includes the CAS registry number, substance name, molecular formula and other information associated with the substances. The second subfile is a property file (D file) containing the type of property, the type and numerical value of property, type and value of parameters, the composition of substance, and others. The third subfile is a reference file (B file) including bibliographic information such as the journal name, author name, title of document and others.

Three subfiles are linked together by unique record key items indicating the substance number (between S and D file) and bibliographic identifier (between D and B file) assigned at data entry. Accordingly, the record of the total data file are structured as shown in Fig. 2. Processing for search and display is carried out with each record as a processing unit.

2.2. *Database Architecture*

The materials database must store a large number of data items which represent both property data and various auxiliary information, therefore a unit record should be very large.

In Fig. 3, principal two techniques for structuring a file and record are presented. In the case 1, source data record for one material species is structured to one logical record, and the total of logical records is compiled to one master file to be the base for search file. Logical records are divided into some physical records to make an inverted file (index file) for search. Each physical record can be restructured into a logical

Table 4. Data items in JICST TH database.

	No.	Data Item	Subfile*	Search Command	Display
Pure Substance (Compound)	1	STARS No.	S	SN	○
	2	Alternative STARS No.	S	---	○
	3	CAS Registry No.	S		○
	4	Preferable CAS Registry No.	S	---	○
	5	Supplementary CAS Registry No.	S	---	○
	6	Chemical Substance Name: STARS Name	S		○
	7	Chemical Substance Name: CA Index Name	S	NM	○
	8	Chemical Substance Name: Synonym	S		○
	9	Chemical Substance Name Fragment	S	FR	×
	10	Molecular Formula	S	MF	○
	11	Number of atoms of each element	S	EL	×
	12	Number of Elemental Species	S	NEL	×
	13	Molecular Weight	S	MW	○
Mixture	14	Mixture Name	D	---	○
	15	Number of Components	D	CNO	×
	16	Constituents	D	SYS	○
	17	Composition	D	---	○
	18	Composition Variables	D	---	○
Property	19	Property: Type	D	same as the code of related property or parameter.	○
	20	Property: Numerical Value	D		○
	21	Parameter: Numerical Value	D		○
	22	Property: Equation	D		○
	23	Applicable Range of Equation	D		○
Auxiliary Information	24	Physical State	D	STATE	○
	25	Pressure State	D	PRESS	○
	26	Feature of Sample	D	---	○
	27	Atmosphere	D	---	○
	28	Measurement Method and Instrument	D	---	○
	29	Error Information	D	---	○
	30	Error in Coefficients of Equation	D	---	○
	31	Deviation of experimental data	D	---	○
	32	Data Type	D	GRADE	○
	33	Date of Evaluation	D	---	○
	34	Abstracter	D	---	○
Bibliographic Information	35	Bibliographic No.	D, B	CN	○
	36	Document Title (English)	B	---	○
	37	Document Title (Japanese)	B	---	○
	38	Language	B	LN	○
	39	Author	B	AU	○
	40	Author Affiliation	B	AA	○
	41	Author Affiliation: Nation	B	NA	○
	42	Document Type	B	---	○
	43	Document ID (Identification)	B	SO	○
	44	Document Name	B	DS	○
	45	Date of Publication	B	PD	○
	46	Publication: Volume, Number, and Pages	B	---	○
	47	Publisher	B	---	○

* Subfile S represents the substance, D the property, and B the reference subfile (shown in Fig. 2) storing the information relevant to the data item.

record by a head directory as a linkage key.

The benefits of this technique (case 1) are the simple record and file structure. However difficulties arise in inclusion of all the information into a logical record.

The case 2 represents the same structure as JICST TH shown in Fig. 2. Source data items of a data category (for example, material identifier) are structured to one logical record and some of these logical records can be edited into a subfile. When some subfiles are prepared, records of a given material in different subfiles can be linked by a unique key. The unique key is A0001 for a material and B0001 for another material as shown in Fig. 3.

Although file construction is complex in this case, this technique has the advantage that the entry of common auxiliary information can be saved for the materials in the master file.

2.3. *Materials Databases Validation and Data Processing*

Materials database must be validated when the following information is sufficiently included in the

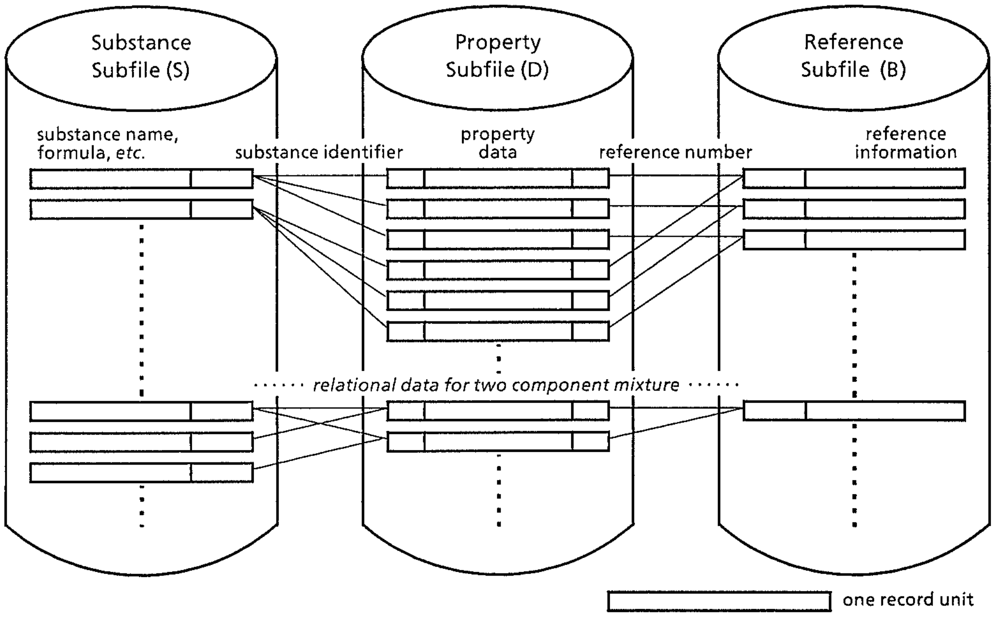


Fig. 2. Structure of records and files in JICST TH database.

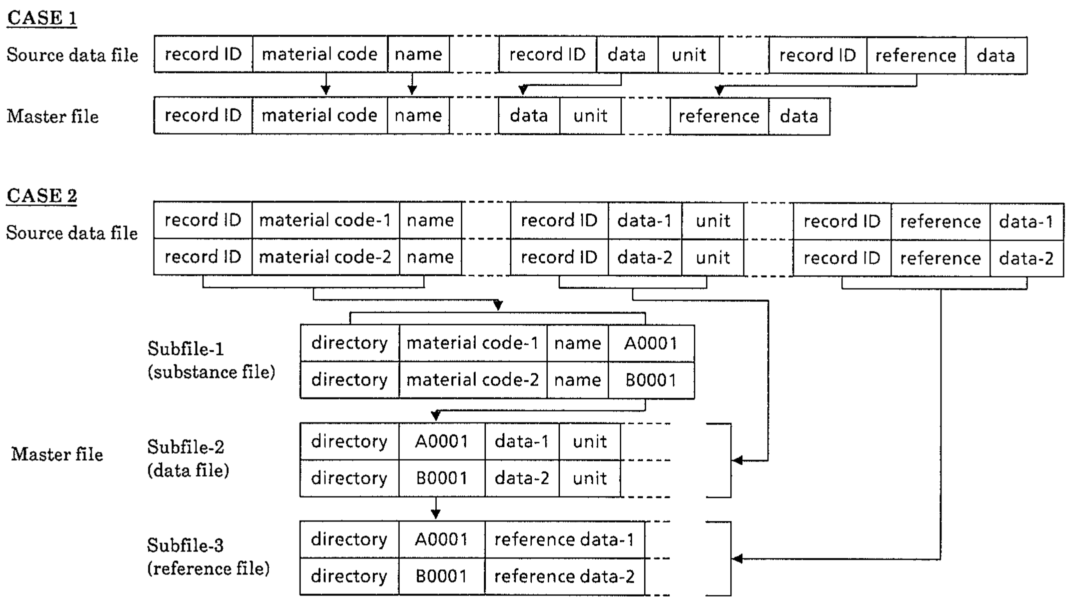


Fig. 3. Record and file structure in JICST TH database.

databases and is standardized: material specifications such as the material name, chemical composition, and production method, as well as material properties such as numerical data, unit, test method and measuring parameters.

The most important problem is the procedure to collect reliable numerical data and maintain their quality. Collection of numerical data from various data sources such as handbooks, data books and documents leads to different description of data. Consideration should be taken into for processing of significant digit of numerical data, unit conversion and various search functions.

In addition, reliability of numerical data is estimated by whether data were evaluated in advance and by whom were described.

Materials databases should contain highly reliable data, but because of large costs and efforts needed for preparing reliable data, a very few data is reliable at present. If these databases can supply high quality data in future, it is believed that the user access will significantly increase.

2.4. *Retrieval System*

Data types of materials databases are represented in simple textual data, numerical data, tables of data, or graphs. Textual data of character mode such as material names, key words, and author names are searchable with full-spelling, right-truncation, and string search techniques. Numerical data can be searched with range searching, above, below, or within the limits specified, to be Boolean searchable.

3. Distribution of Materials Databases

Distribution systems of materials databases are changing with development of computer and communication technology as well as storage media. One of the most useful distribution media is the on-line database system that enables distant users to search, retrieve and display the desired data with a microcomputer, phone-line and CRT terminal.

The system contains a computer hardware for information processing, database management system, communication and networking system for the distribution of databases.

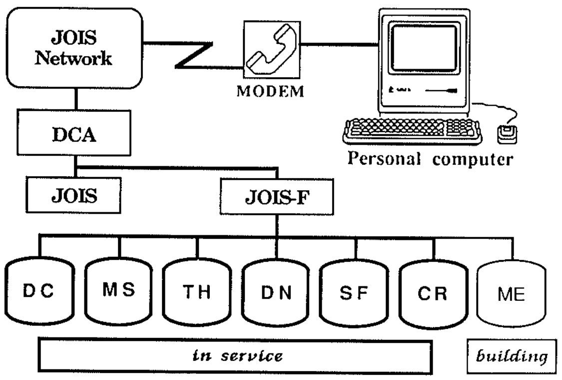
Only a few systems provides graphical output of numerical data or display of pictorial information which needs a high level database management system. Users demand that materials databases include a large number of materials and properties, but really only small, specialized databases of limited coverage are available. Since no all-around database satisfying various users is available, strong demands arise for interlinking among the separate databases to form an integrated system which allows to use some databases by one access.

There are some integrated systems such as CIS (Chemical Information System) and JOIS-F (JICST Online Information System-Factual database). Feature of JOIS-F is presented in Fig. 4.

The JOIS-F system now provide six factual databases and in the near future one more database will be in service as shown Fig. 4.

Chemical databases such as MS, TH, CR, SF and DC are linked together through a unique substance code by which these chemical databases are cross-file searchable, though the individual databases are controlled by independent database management systems.

The JOIS-F system supports many kinds of search, Boolean logic and some graphic display facilities, but other functions such as high graphic and pictorial display, data manipulation, statistical data analysis, and the other application softwares are not satisfactory.



DC: Chemical Dictionary Database
MS: Mass Spectral Database
TH: Thermophysical and Thermochemical Property Database
DN: DNA Database
SF: Chemical Substance Safety Regulation Database
CR: Crystal Structure Database
ME: Materials Strength Database for Engineering Steels and Alloys

Fig. 4. System configuration of JOIS-F.

Users demand for downloading of data into their desktop microcomputer systems are increasing. Data once downloaded into a microcomputer can be combined with user's private data or its own application softwares, and then its own small systems will be built and the data are used in CAD/CAM or other operations.

In addition, the development of data storage media has permitted to make data packages on floppy disks or CD-ROM together with various softwares for manipulating the data.

Worldwide networking such as STN International and DIALOG is now available. Gateway systems which save various log-on procedures to many on-line systems have been developing.[40,41] There are two types of gateway system; one type uses a host computer switching many existing on-line systems and another permits a user to perform the same procedure on its own terminals by using communication softwares.

4. Future Aspect

Although some on-line systems providing various materials databases are available at present, standardization is not satisfactory in terms of commands, protocols, data form, definition and nomenclature, *etc.* Therefore it is troublesome for users to access useful databases in different systems.

Progress of networking and gateway system will promote standardization of protocols and permit easy access of users to many systems and databases.

These developments of telecommunications will stimulate uniformity of specifications such as materials nomenclature, testing method and data form.

Moreover, it is hoped that the reference database can be an interface to materials, testing conditions and property data connecting with various reference information such as data sources and testing organizations.

In the future, computer-based information sources will be directly utilized in combination with computer-aided design (CAD), manufacturing (CAM), and testing (CAT) systems.

Expert systems for estimating materials properties such as a metal database developed by University of Syracuse[42,43] and AMDADS (AiResearch Materials Data Analysis and Dissemination System) by AiResearch Manufacturing Co.,[44] are in application.[45,46] To obtain most suitable information easily in materials databases having complicated data structure, establishment of expert systems is hoped interfacing to materials databases.[47]

In MEDDBASE (Materials Engineering Design Data BASE) within the AMDADS frame, the program leads the user through the various choices of materials configuration descriptors (menus) in automatic mode. To include the best known information with appropriate qualifier where no sanctioned design data were available, each material property value is identified by one of the codes; "A representing at least 99 % of the population of values is expected to equal or exceed this value with 95 % confidence ".

Since adequate estimation of complicated materials properties is very difficult, research and development in computer application technology filed will give us many challenging subjects.

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