MITS 2008 *Materials Information & Technology Solutions* **MITS 2008** *Materials Information & Technology Solutions* **MITS 2008** *Materials Information & Technology Solutions*

MITS 2008

July 17 (Thu) - 18 (Fri), 2008

International Symposium on Materials Database

Organized by

Materials Database Station (MDBS)
National Institute for Materials Science (NIMS)

Venue

Tsukuba International Congress Center
2-20-3, Takezono, Tsukuba, Ibaraki, 305-0032, Japan

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Contents

International Symposium on Materials Database
MITS 2008

Date: July17 (Thu)-18(Fri), 2008

Venue: Tsukuba International Congress Center

(EPOCHAL TSUKUBA)

July 17 (Thu)   At Convention Hall 200

8:45-9:00 Opening Remarks

Session 1 (9:00~10:30)

Chair: Prof. Tatsuo Sakai, Ritsumeikan University, Japan

9:00~9:30 **New Aspects of Knowledge on Materials and Required Databases**

Dr. Munetsugu Matsuo, National Institute for Materials Science (NIMS), Japan

9:30~10:00 **The Role of Materials Metrology and Eco-design in Materials Property Databases**

Dr. Graham D Sims, National Physical Laboratory, UK

10:00~10:30 **Business Model of Internet-based Material Database: MatWeb**

Dr. Nils A. Steika, Automation Creations Inc., USA

Session 2 (10:45~12:15)

Chair: Dr. Pierre Villars, Materials Phases Data System, Switzerland

10:45~11:15 **Structuring Knowledge of Nanomaterials and Nanorisks**

Prof. Yukio Yamaguchi, University of Tokyo, Japan

11:15~11:45 **NIST Databases for Inorganic-Materials Research**

Dr. Terrell A. Vanderah, National Institute of Standards and Technology (NIST), USA

11:45~12:15 **Database to Use Materials in High Quality**

Dr. Koichi Yagi, National Institute for Materials Science (NIMS), Japan

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Session 3 (13:30~15:30)

Chair: Dr. Graham Sims, National Physical Laboratory, UK

13:30~14:00 **Materials Database Project in KOREA**

Dr. Byoung-Kee Kim, Korea Institute of Materials Science (KIMS), Korea

14:00~14:30 **Construction of Materials Databases and Their Useful Application in the Society of Materials Science, Japan(JSMS)**

Prof. Tatsuo Sakai, Ritsumeikan University, Japan

14:30~15:00 **Current Status and Future Prospect of Materials Data Sharing in China**

Prof. Haiqing Yin, University of Science and Technology Beijing, China

15:00~15:30 **Indian Materials Database for Scientists, Engineers and Industries**

Dr. R.K.Dayal, Indira Gandhi Centre for Atomic Research, India

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Session 4 (16:00~17:30)

Chair: Dr. Yibin Xu, National Institute for Materials Science (NIMS), Japan

16:00~16:30 **Data-Driven Materials Design using Pauling File Binaries Edition**

Dr. Pierre Villars, Material Phases Data System (MPDS), Switzerland

16:30~17:00 **Finding Materials for Transformation Toughening through Datamining**

Dr. Marcel H.F. Sluiter, Delft University of Technology, the Netherlands

17:00~17:30 **Inference from Various Material Properties Using Mutual Information and Clustering Methods**

Proposal of the XML Specification as a Standard for Materials Database Query Submission and Result Retrieval

Dr. Emre Tasci, Delft University of Technology, the Netherlands

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July 18 (Fri)   At Conference Room 303

Panel Discussion (9:30~11:30)

Chair: Dr. Masaki Kitagawa, National Institute for Materials Science (NIMS), Japan

9:30~11:30 **Sustainability and Materials Database**

New Aspects of Knowledge on Materials and Required Databases

Munetsugu MATSUO [1*]

[1] Materials data base station, National Institute for Materials Science (NIMS), 2-2-54 Nakameguro, Meguro-ku, Tokyo 153-0061, Japan
* Corresponding author's e-mail address: MATSUO.Munetsugu@nims.go.jp

Hierarchy of materials information

The famous talk "There's Plenty of Room at the Bottom"[1] by Nobel Physics Laureate Richard Feynman at 1959 implies hierarchy of the knowledge on materials consisting of the bottom-up structure of macroscopic, microscopic and nano-scale information, as shown in Fig.1. In construction of databases we must take into account that the needs of materials information varies with users, producers, and researchers of materials and design to meet for the needs. Integration and correlation of the databases of different levels in the hierarchy should be considered:

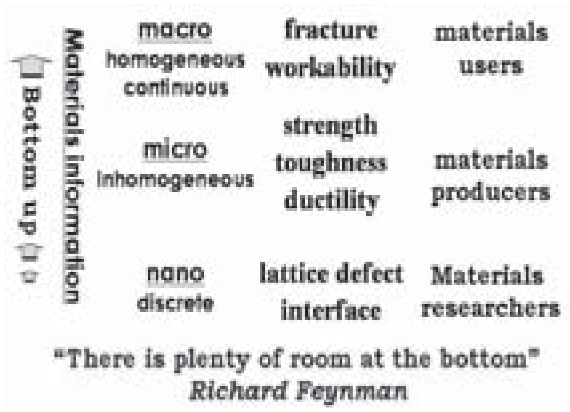


Fig 1 Hierarchy of materials knowledge

MSE Tetrahedron

The knowledge on materials science and engineering are conventionally represented as a tetrahedron[2]. Four corners of the MSE tetrahedron correspond to the elements of the essential information of materials; performance, property, structure and processing. Trends of the production and utilization of materials under dynamic and extreme states require a new scope of knowledge such as shown in Fig.2.

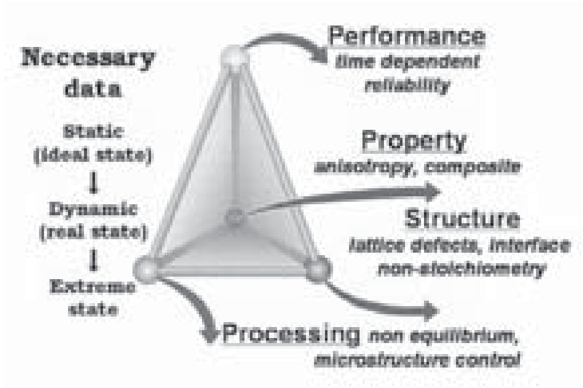


Fig 2 A new version of MSE tetrahedron

Ensuring High Reliability

Reliability is essential to databases: and means for ensuring the reliability should be developed: a possible way is to employ effectively the data of citations: the numbers and details of the citing literature will help the user of database for evaluating validity of the data contained.

NIMS diffusion database

Plans for actualization of the above considerations will be presented with reference to NIMS diffusion database.

References

[1] R. Feynman: Engineering and Science, .23(1960), February, 22.

[2] M. Flemings: .Ann. Rev. Mater. Sci., 29(1999), 1.

New Aspects of Knowledge on Materials and Required Databases

Munetsugu MATSUO

NIMS Database Station

My Favorite

Quotations

from

Eminent Scientists

Referring to

"Knowledge on Materials"

"To understand function, study structure"

Francis Crick

Co-discoverer of the double helix structure of DNA

"Everything is made of atoms"

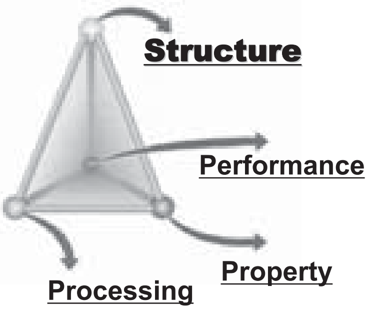
Richard Feynman

"When we have some control of the arragement of things on a small scale, we will get an enormously greater range of properties"

Materials Science and Engineering Tetrahedron (after M.F. Flemings and S.M. Allen)

Structure

Topmost among Four Elements of "Knowledge on Materials"



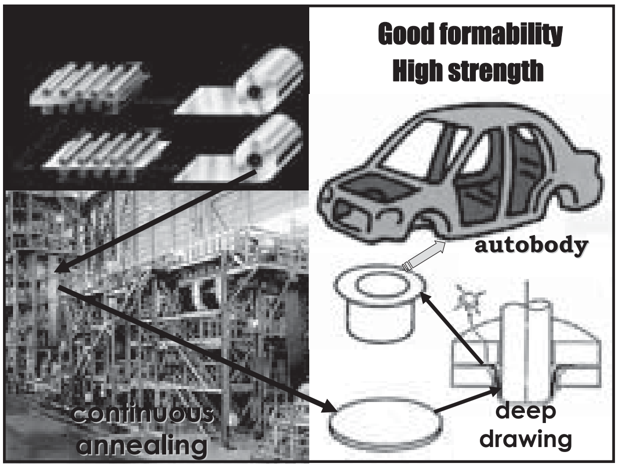
Needs for nontraditional knowledge

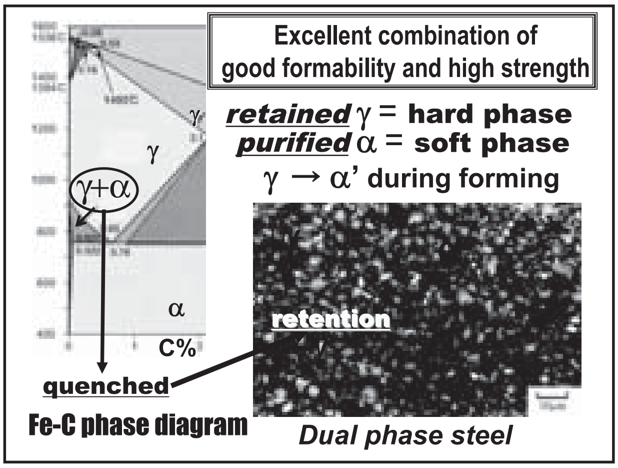
(my personal experiences)

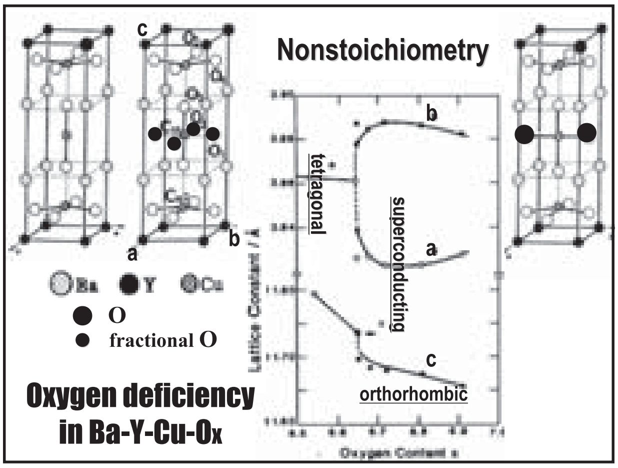
① Nonequilibrium

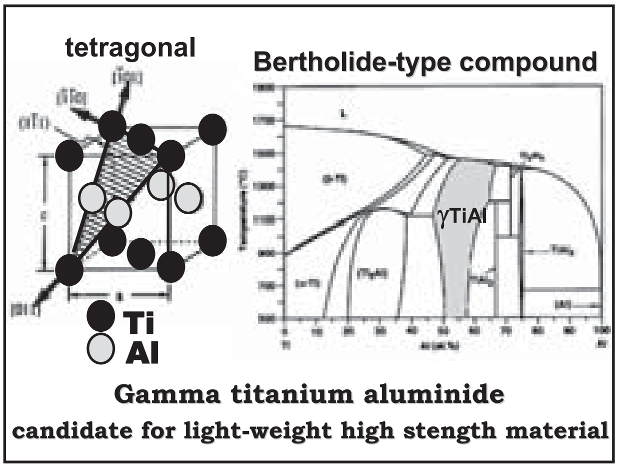
② Nonstoichiometry

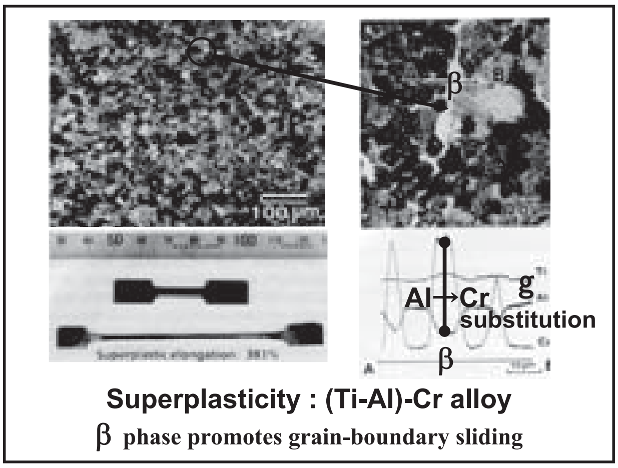
③ ① plus ②

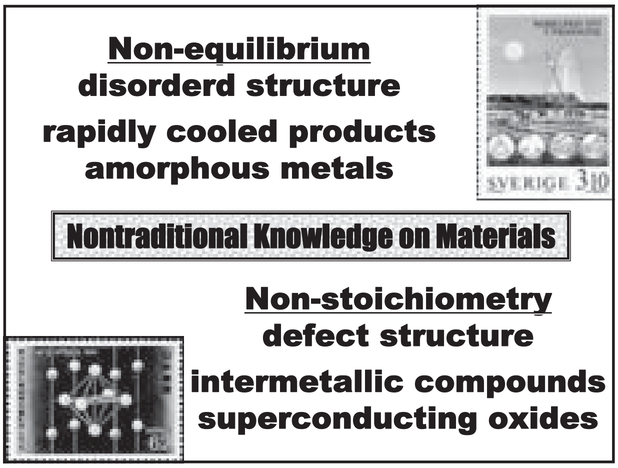

Good formability
High strength
autobody
deep
drawing
continuous
annealing

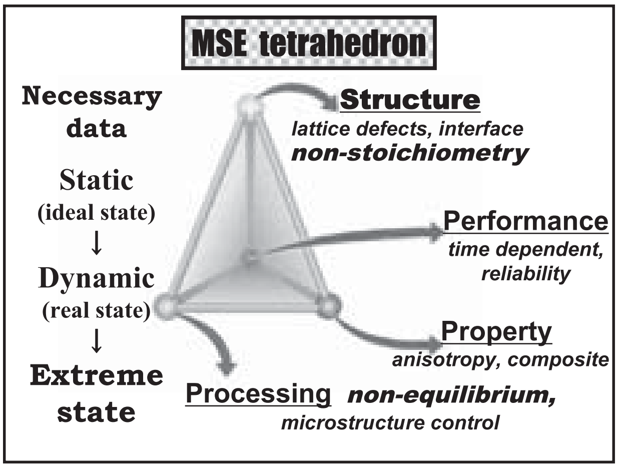

Excellent combination of
good formability and high strength
retained γ = hard phase
purified α = soft phase
γ → α' during forming
γ
γ+α
α
C%
retention
quenched
Fe-C phase diagram
Dual phase steel

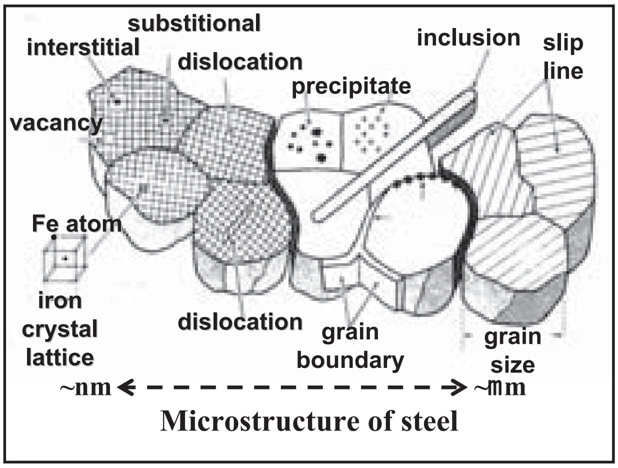

Nonstoichiometry
c
a
b
tetragonal
superconducting
orthorhombic
Ba Y Cu
O
fractional O
Lattice Constant / Å
Oxygen Content x
Oxygen deficiency
in Ba-Y-Cu-Ox


tetragonal
Bertholide-type compound
γTiAl
Ti
Al
Gamma titanium aluminide
candidate for light-weight high stength material


β
100 μm
Al→Cr
substitution
g
β
Superplasticity : (Ti-Al)-Cr alloy
β phase promotes grain-boundary sliding


Non-equilibrium
disorderd structure
rapidly cooled products
amorphous metals
SVERIGE 310
Nontraditional Knowledge on Materials
Non-stoichiometry
defect structure
intermetallic compounds
superconducting oxides





Hierarchy of materials information

Materials information — Bottom up

viewpoints	interests	needs
macro homogeneous continuous	fracture workability	materials users
micro Inhomogeneous	strength toughness ductility	materials producers
nano discrete	lattice defect interface	materials researchers

"There is plenty of room at the bottom"
Richard Feynman

Database as a treasury and an enlarged intimate supplement to "Knowledge on Materials"

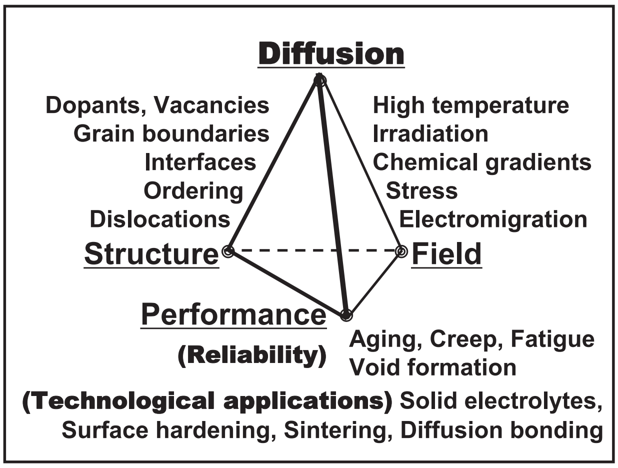
⇕

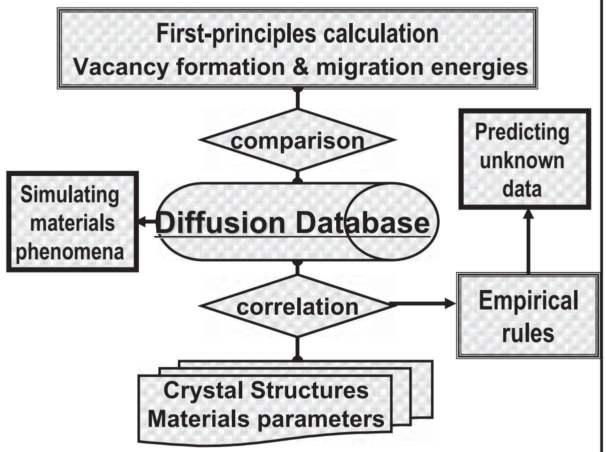
incorporation of current needs for nontraditional knowledge

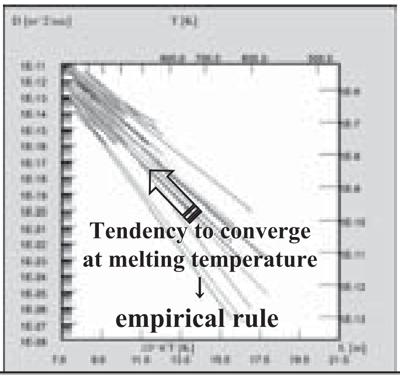
Construction
of
Databases Incorporating

Nontraditional Knowledge on Materials

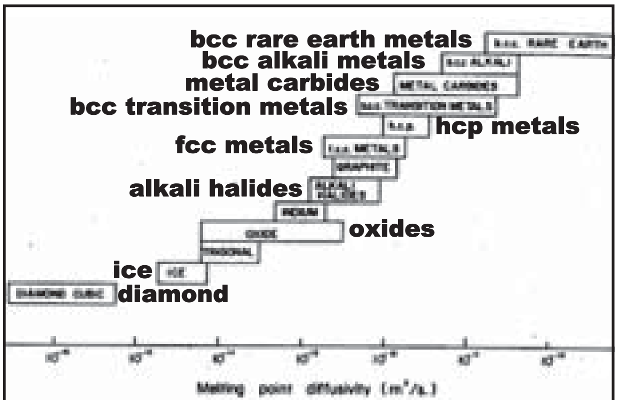
Particularly important is
the knowledge of diffusion relevant for kinetics of materials processes





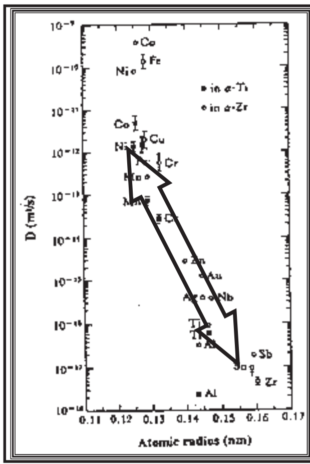


Arrhenius plots of copper diffusion data
In NIMS Diffusion Database



Melting point diffusivity of materials

By Brown & Ashby



Data analysis
with reference to
crystal structure DB

↓

Correlation between
diffusion rate and
diffusant atomic radius
in α-Ti and Zr

↓

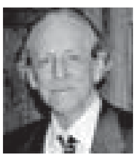
New empirical rule

How to assure the reliability of data?

Citations as an effective tool
for evaluation of stored data.

How many times the data are cited?

How the data are referred and compared?



Eugene Garfield

Ideal of materials database
--- "As we may think" ---

amplification of knowledge

creation of associative trail

assurance of reliable knowledge

The Role of Materials Metrology and Eco-design in Materials Property Databases

Graham D Sims

National Physical Laboratory, Industry and Innovation Division,
Teddington, Middlesex, UK, TW11 0LW

- Corresponding author's e-mail address: graham.sims@npl.co.uk
-

Abstract

If databases are to valuable in design, then designers must have confidence in the data. The precision of the data can be particularly important when 'A' and 'B' design values are used, resulting in unacceptably low design values if the data set has high scatter. In addition to the basic material properties, there is increasing interest in eco-design information related to the energy and material usage throughout the product life cycle.

An initiative undertaken by VAMAS (Versailles Project on Advanced Materials and Standards) to improve the precision and reliability of the measurement of material properties by ensuring best practice in metrology is applied to these measurements is described. Material properties can be divided into those that are considered to be intrinsic (sometimes referred to as inherent or fundamental) and procedural depending on the characterisation method used. The work undertaken by a CIPM Working Group on Materials Metrology is reported, including the recommendations for further work. The potential impact of a formal collaboration between VAMAS and BIPM (Bureau International des Poids et Mesures) on the quality of material properties reported.

This paper reviews also the result of a recent survey in the UK of the needs related to the supply of material data and the use of material databases. It was found that a wide range of data covering mechanical, electrical, thermal and environmental properties are required. A useful number of respondees were prepared to donate short-term data to a central database.

Business Model of Internet-based Material Database: MatWeb

Nils A. Steika[1*], Dr. Dale O. Kipp[1]

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Blacksburg, VA 24060, USA
*email: nils.steika@matweb.com

Introduction:
MatWeb has successfully built a reputation as a reliable source, and a key part of the materials selection process. Over the past several years, the material selection process has become more computer and internet driven. The availability of online information, coupled with increased ease of data collection and updates, has supplanted decades of handbook-driven and experience-driven material selection. Many internet databases using various business models have had success in providing information to engineers and designers choosing the materials to use in their products. Subscription-based, government supported, and free Internet databases have all proven to be capable of meeting the needs of today's tech-savvy engineers. The MatWeb materials database was initiated in 1996 to capitalize on advances in information delivery technology, to provide a resource of technical data used for materials screening and selection. MatWeb's business model is to (1) provide a broad array of materials, (2) allow free access to data for all users, (3) have a high level of user friendly search tools, and (4) be financially supported by advertising on the website. This model has made MatWeb the busiest web site for materials data, serving over 23,000 users each weekday. This large audience of engineers makes our business appealing to other materials related companies that wish to reach them with their message. This talk will examine the roles and capabilities of MatWeb and some other potential Internet materials database business models that have proved successful.

Technology:
When running a website, there is always a need to keep up with changing programming languages. There is a steady stream of improvements to the computational efficiency of the code. MatWeb recently underwent extensive upgrades: (1) New servers power the site so we can handle the large number of searches per day, (2) the back end of MatWeb is a normalized SQL Server database that was redone to handle conditional data and speedier searches, and (3) the data base is accessed with ASP.NET and AJAX programming. (an upgrade from ASP Classic). The search features of MatWeb have grown along with the data. Our qualitative text search engine can parse multiple words and prioritize matches based on the location of the terms in various data sheets. Quantitative searches allow our users to search with property or composition data. There are also tools available to registered users that allow combinations of text-based, category-based, property-based searches, and conditional data searches. Registered users also can use features like side-by-side comparisons, and export of the data in a variety of useful formats including Excel, SolidWorks, ANSYS, COMSOL, and others.

Searchable Database:
The heart of MatWeb is its collection of data, currently consisting of over 67,000 technical data sheets. The data is collected on a continual basis, only from verified sources: 90% manufacturers, 10% literature, handbooks, and professional societies. This makes the data reliable, which is vital to the usefulness of any data collection. The original sources are referenced on the datasheets so that users can research additional information or clarification if required. MatWeb's data sheets are categorized into systematic categories and contain text explaining key attributes and applications, and on average about 20 numerical data points. MatWeb's staff adds over 10,000 data sheets per year, and updates its

content on a regular basis. The original MatWeb data sheets tracked only a single data point (stored in a metric unit) for 100 possible properties. MatWeb now tracks ranges or multiple instances of properties for each material, selecting from over 1000 possible physical properties, and stores data points in the units received. The newest feature of MatWeb is the ability to store and search on conditional data (multi point curves, etc).

MatWeb
MATERIAL PROPERTY DATA

Business Model of Internet-based Material Database: MatWeb

Nils A. Steika
MatWeb Division, Automation Creations, Inc.

MITS 2008 International Symposium
Tsukuba Japan
July 17, 2008

AUTOMATION CREATIONS, INC.

MatWeb
MATERIAL PROPERTY DATA

Introduction

- Business Model:
  - Large collection of data
  - Easy, free access to data
  - Helpful search tools
  - Revenue from advertising
- Technology used
- Challenges faced
- Future growth

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MatWeb
MATERIAL PROPERTY DATA

Collection of Data

- Reproduce data from manufacturers at no cost to them
  - 90% of MatWeb data from > 620 Manufacturers
  - Remaining from Handbooks, Professional Societies
- Broad range of materials
  - Ceramics
  - Metal alloys
  - Polymers
  - Composites
  - Fluids
  - Wood
  - Fibers
  - Pure Elements
- Over 68,000 Material Datasheets, and 1,102,000 data points

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Sample datasheet

DuPont Teflon® PTFE 7C Granular Molding Powder

Categories: Polymer; Thermoplastic; Fluoropolymer; PTFE

Material Notes: Teflon® PTFE white granular molding powders are ideal for molding many different end products and stock shapes. Excellent chemical resistance, electrical properties, high temperature performance, low temperature toughness, plus unique adhesion and flame resistance.

Teflon® PTFE granular molding powders are processed by compressing them into a desired shape and heating them at temperatures above their melting point to consolidate the powder.

Resin Characteristics: Small, fibrous particles with a low bulk density Uses: Usually mixed with inorganic powders to make filled molding compounds that offer improved wear and cold flow resistance.

Typical properties for Teflon® PTFE Granular Resin.

Data provided by the manufacturer.

Key Words: Polytetrafluoroethylene; DuPont Fluoroproducts

Vendors: **Click here to view all available suppliers for this material.**

Please click here if you are a supplier and would like information on how to add your listing to this material.

Printer friendly version | Download as PDF | Download to Excel (requires Excel and Windows) | 3/28

Physical Properties	Metric	English	Comments
Specific Gravity	2.16 g/cc	0.0780 lb/in³	ASTM D4894
Bulk Density	0.250 g/cc	0.00903 lb/in³	ASTM D4894
Water Absorption	<= 0.0100 %	<= 0.0100 %	24 hours; ASTM D570
Particle Size	28.0 µm	28.0 µm	ASTM D4894
Linear Mold Shrinkage	0.0600 cm/cm	0.0600 in/in	at preform pressure of 35 Mpa; ASTM D4894

Mechanical Properties	Metric	English	Comments
Hardness, Shore D	50.0 - 65.0	50.0 - 65.0	ASTM D2240
Tensile Strength, Ultimate	37.9 MPa	5500 psi	ASTM D4894
Elongation at Break	400 %	400 %	ASTM D4894
Flexural Modulus	0.496 GPa	71.9 ksi	ASTM D790

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Sample datasheet

Electrical Properties	Metric	English	Comments
Volume Resistivity	>= 1.00e+18 ohm-cm	>= 1.00e+18 ohm-cm	ASTM D257
Surface Resistivity per Square	>= 1.00e+18 ohm	>= 1.00e+18 ohm	ASTM D257
Dielectric Constant	2.10	2.10	1MHz; ASTM D150
Dielectric Strength	18.0 kV/mm	457 kV/in	100 micrometers film; ASTM D149
Dissipation Factor	<= 0.000100	<= 0.000100	1MHz; ASTM D150
Arc Resistance	>= 300 sec	>= 300 sec	ASTM D495

Thermal Properties	Metric	English	Comments
Melting Point	317 - 337 °C	603 - 639 °F	ASTM D4894
Flammability, UL94	V-0	V-0	
Oxygen Index	>= 95.0 %	>= 95.0 %	Limiting Oxygen Index; ASTM D2863

Processing Properties	Metric	English	Comments
Drying Temperature	379 - 429 °C	714 - 804 °F	Cure Temperature

Descriptive Properties	
20% Hydrochloric Acid Transmission, g/100sq in.	<0.01
50% Sodium Hydroxide Transmission, g/100sq in.	< 01
Acetic Acid Transmission, g/100sq in.	0.41
Acetone Transmission, g/100sq in.	0.95
Acetophenone Transmission, g/100sq in.	0.5
Benzene Transmission, g/100sq in.	0.64
Carbon Tetrachloride Transmission, g/100sq in.	0.31
Chemical/Solvent Resistance	Excellent
Detergent Resist. on grit-blasted aluminum, Hours	624
Detergent Resistance on aluminum, Hours	264
Detergent Resistance on grit-blasted steel, Hours	24
Ethyl Acetate Transmission, g/100sq in.	0.76
Folding Endurance, # cycles, .18-.20 mm	>10^6

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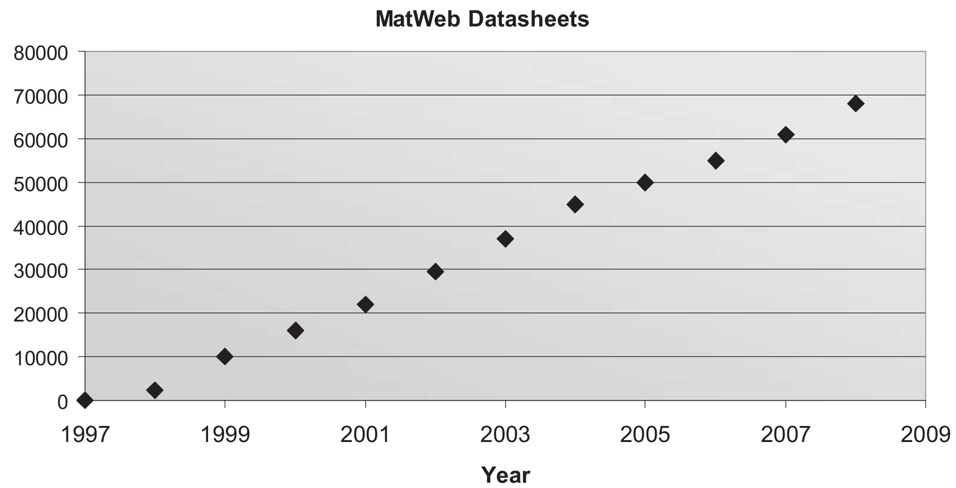
Growth of data

- Steady addition of new material data: 5,000-8,000 new each year



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Accessibility of Data

- Free, online, anonymous access
- 23,000 users per weekday; 360,000 per month
- Free registration for advanced searching, other tools
- 240,000 registered users
- Option to pay $75U.S. for advanced storage and export functions

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Search Tools

- Qualitative
  - Full text, keywords
  - Index pages: Category, Trade name, Manufacturer
- Quantitative
  - Property, composition
  - Conditional data
- Specific pages
  - UNS number
  - Lubricants, Polymer Films

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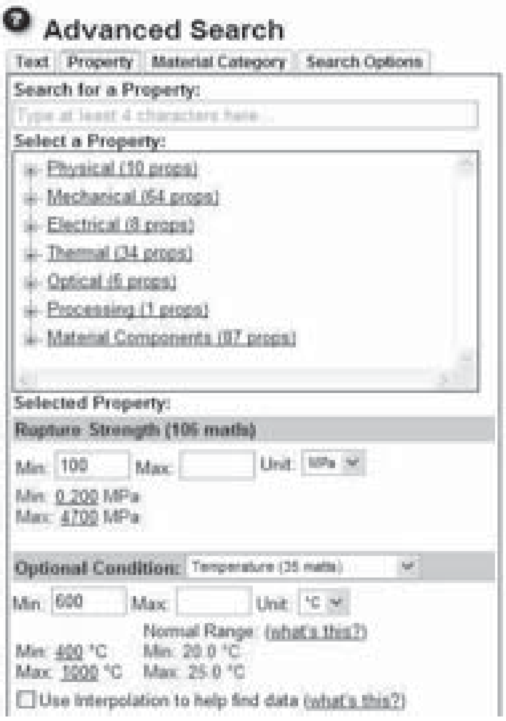
Advanced Searching



- Combine text, category, and property criteria to refine search
- Conditions further refine results

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MatWeb
MATERIAL PROPERTY DATA

Secondary Features

- Personal Folders: Material storage, and editing
- Data transfer capability to CAD/FEA programs
- Additional tools for users
  – UOM converter
  – Technical Glossary
  – Weight, inertia calculators

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MatWeb
MATERIAL PROPERTY DATA

Advertising supported

- 70% of MatWeb revenue from advertising
- Large user base is technical/engineering fields oriented group
- Materials industry desires to reach that audience
  - Listings on datasheets
  - Banners on main pages
- Online advertising becoming more desirable than print

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Programming Technology

- Began in 1997 with HTML site that hit several Microsoft Excel worksheets
- Moved to Microsoft Access database in 1998, ASP coded website
- In 2000 MatWeb went to SQL, ASP served pages
- Total rewrite in 2007

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MatWeb
MATERIAL PROPERTY DATA

Current Technology

- Dedicated SQL server
  - Enterprise level database
  - Handles large quantity of data, many concurrent users
  - Fast, full text searches
- ASP.NET
  - Supports high traffic
  - AJAX tools allow fast communication between website and database
  - Friendly user experience
  - Security, error trapping

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Current Technology, con’t

- Multi-threaded search code
- Data stored in native units, converted on the fly for display
- Over 1000 properties tracked
- Interpolated data created for searching purposes

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MatWeb
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Key Relationships

- FEA/CAD Partners
  - SolidWorks, ALGOR, ANSYS, COMSOL, Engrasp
- Collection of Data
  - NIMS, RTP Company, Equistar Chemicals, Bamberger Polymers
- Data transfer and storage
  - MatML and Materials Digital Library
- Installation of MatWeb on other sites
  - Quadrant, FotoFab, others

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MatWeb
MATERIAL PROPERTY DATA

Challenges with this model

- Pressure to maintain and grow data
  - Stay largest, most comprehensive
- Attracting new users, new advertisers
  - Revenue depends on it
- Database infiltration
- Data theft
  - IP address blocking, other security measures

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Future Growth

- Expand international data
- Support for multiple languages
  - asia.matweb.com
- Expand non-linear data
- Adding support for graphical display of data
- Graphical search support

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MatWeb
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Summary

- MatWeb fills a need for low cost/high volume data source
- MatWeb's broad, reliable data collection and useful search tools serve over 23,000 users per weekday
- The large user base makes us an appealing advertising option for materials industry
- MatWeb continues to grow and collaborate to meet user's needs

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- Thanks to Yamazaki Masayoshi, Dr. Teruo Kishi, and NIMS for the invitation to speak here

- Questions?

Nils Steika
Email: nils.steika@matweb.com

Structuring Knowledge of Nanomaterials and Nanorisks

Yukio Yamaguchi and Yasuto Matsui

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The main objective of structuring knowledge is to stimulate new ideas for understanding nanomaterials in ways that strongly relate processes, nanostructures, functions and applications. People in industry are concerned about solutions to problems when developing products and want to gain generalized knowledge. It is necessary to match industrial problems with generalized academic knowledge in a timely manner. Although material scientists focus on differences in material characteristics, the formation of the nanostructures of advanced materials can be unified conceptually with mechanism-oriented knowledge. We can offer a methodology to structure knowledge for deep understanding of the relationships among processes, structures and functions. The key is to elucidate the mechanisms of nanostructure formation, such as clustering, nucleation and micro-phase separation that occur in various types of fabrication processes. New ideas based on structured knowledge eventually result in technological innovation [1].

The purpose of structuring knowledge of nano-risks is to search out the risk factors of nanomaterials through our software which can reveal the potential risks. The risk assessment platform consists of three domains as shown in Fig.1.

Fig.1: Schematic relationships among nano-materials, exposure assessment and hazard identification built in the platform of structuring knowledge.

References

[1] Y.Yamaguchi, S.Noda and H.Komiyama, Chemical Engineering Letter, in press.

Structuring Knowledge of Nano-Materials and Nano-Risks

Yukio Yamaguchi
Department of Chemical System Engineering,
The University of Tokyo

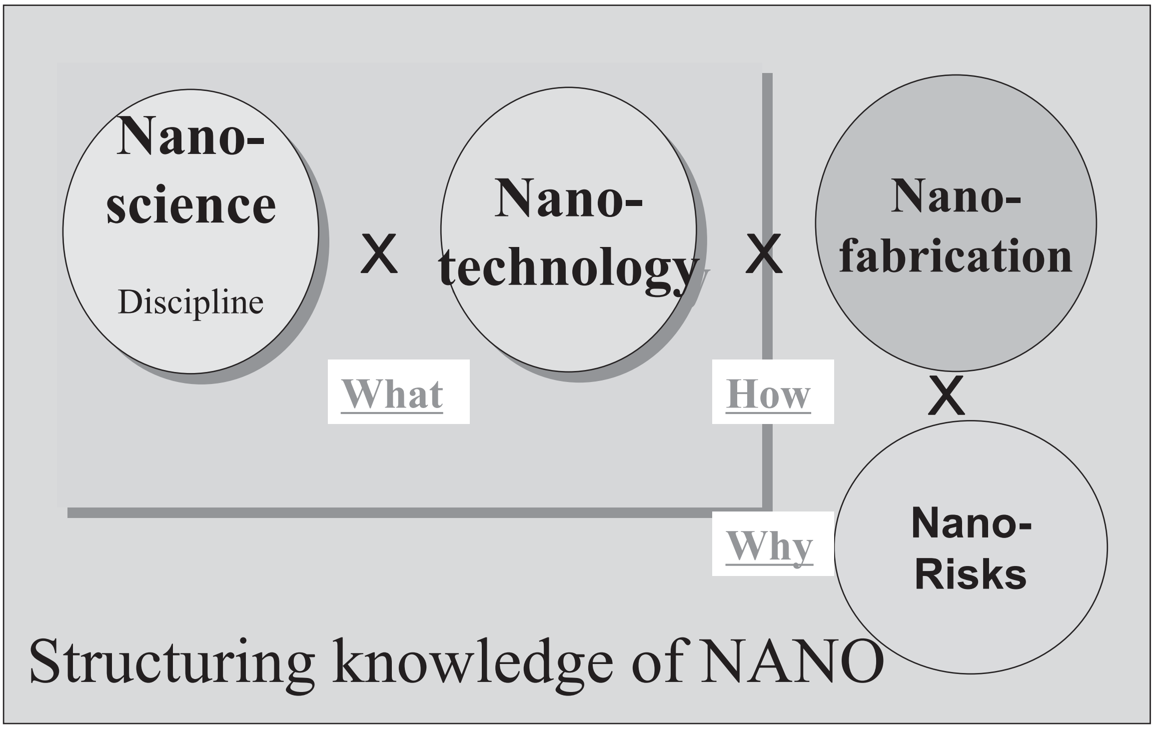
Objective

We develop a knowledge platform to search information and to obtain some criteria index for nano-risks, which closely linked to nano-materials.

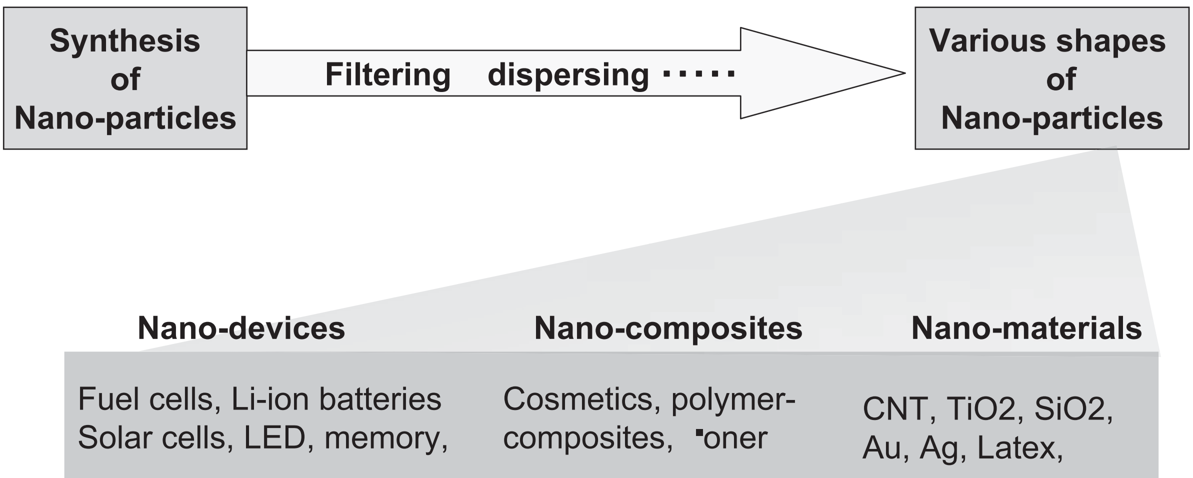
- Prototype platform available April, 2009

2

Toward innovation



Nano-materials have substantial potential to solve environment-energy related issues by changing the higher-order structures.



Variation of Nano-particles

- Metals: Au, Ag, Pt, Ti, Cu,････
- Metal Oxides: SiO_2 , TiO_2, ZnO,････
- Polymers: latex, toner, ････
- Organics: pigments, surfactants, ････
- Carbons: Fullerene, CNT, CB, CF,･･･

There are infinite kinds of nanoparticles.

How can we check them?

Characteristics of Nano-materials

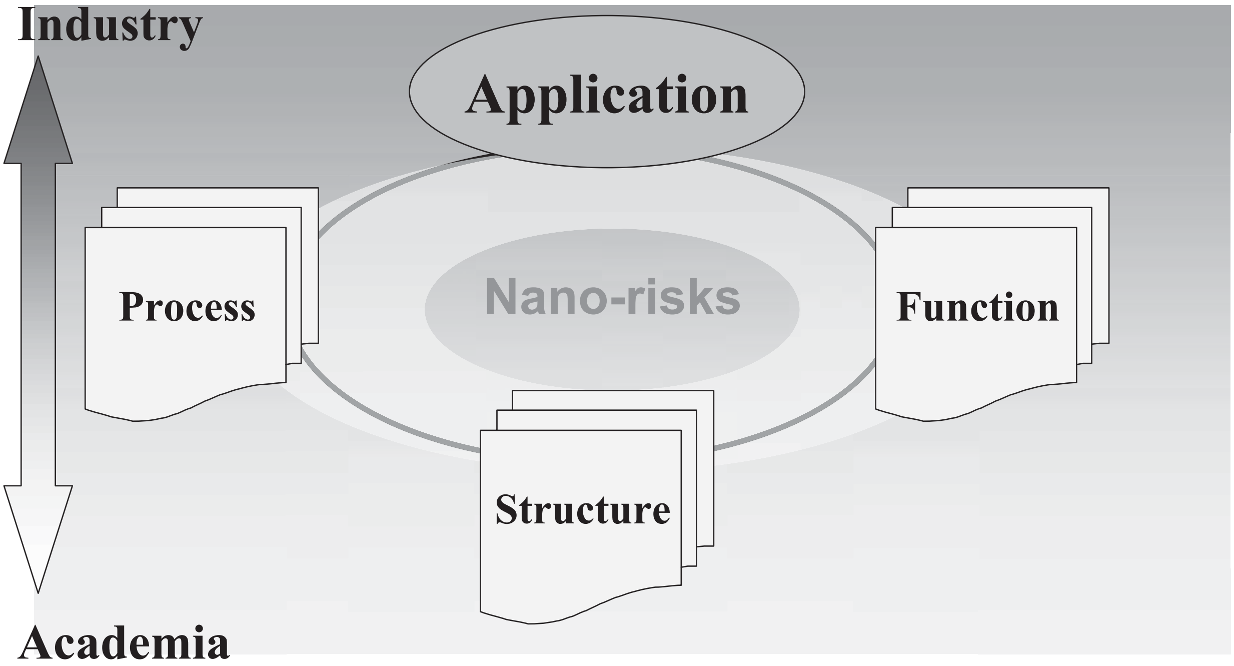
Chemical issues

- Huge surface area
- Easy to aggregate
- Higher dissolving rate if it dissolves
- Higher amount of adsorbents
- Higher activity as catalysts
-

Physical issues

- Needle-like shapes
- Penetration to cells if the size is smaller
- Aggregates are trapped in organs
-

Platform for Innovation



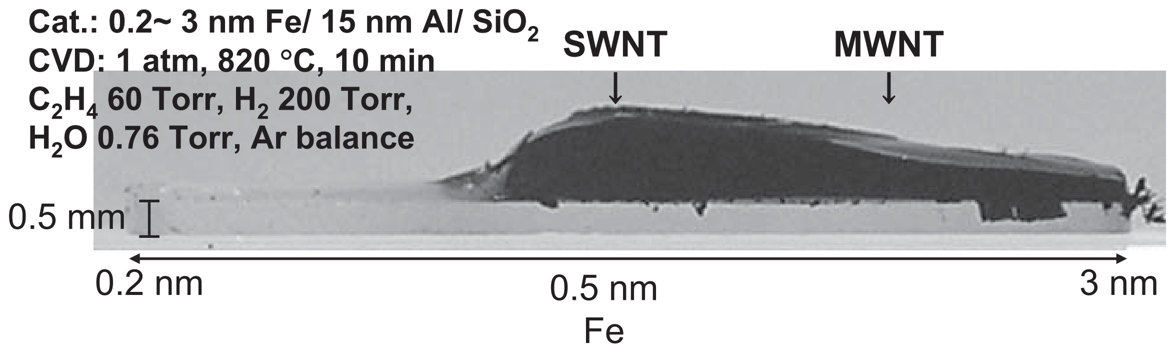
Y.Yamaguchi, S.Noda, H.Komiyama, Chemical Engineering Comm. ***in press***

Examples of Nano-materials

NANO are crucial materials for environment and energy issues.

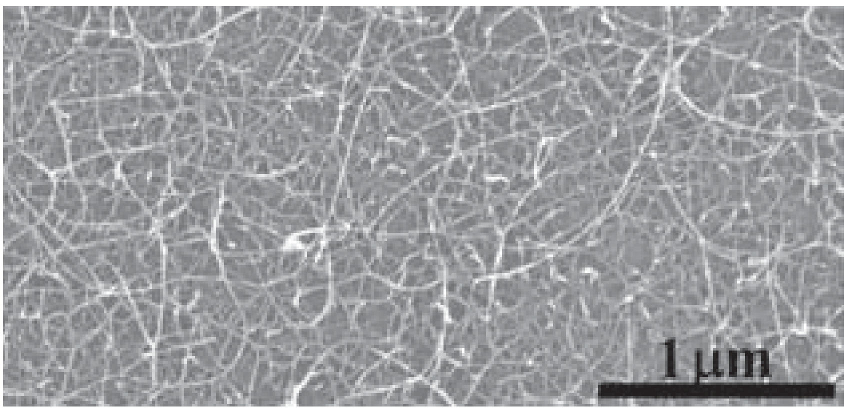
Production process of CNT

Catalyst and CVD



Transparent Electrodes

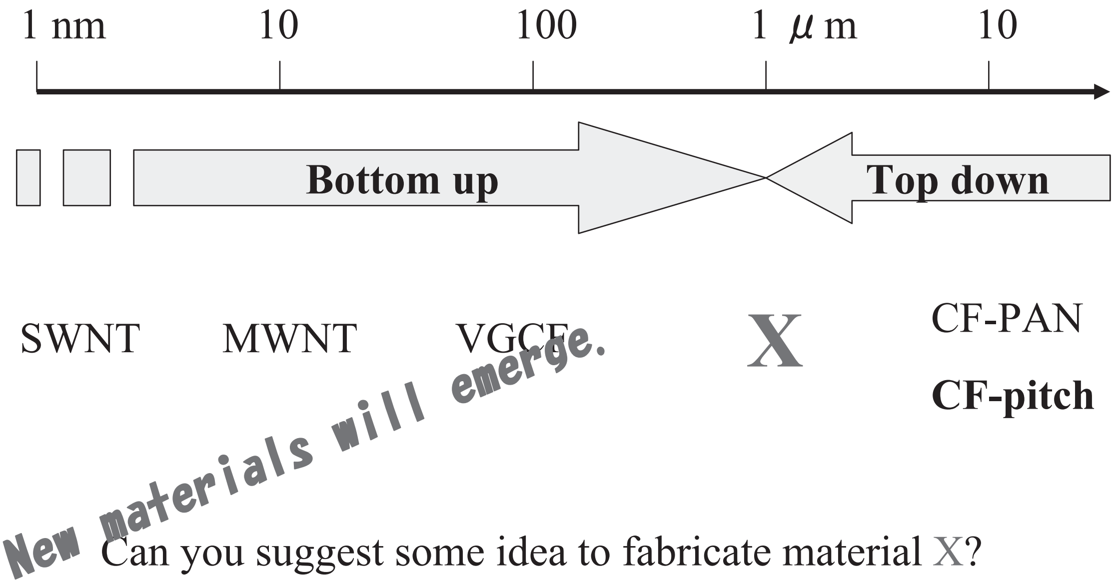
Tailored SWNT networks show good property.



Optical transmittance: 94 %, Sheet resistance: 1.9 kΩ/□

New types and shapes of nano-materials will emerge.

Carbon Materials

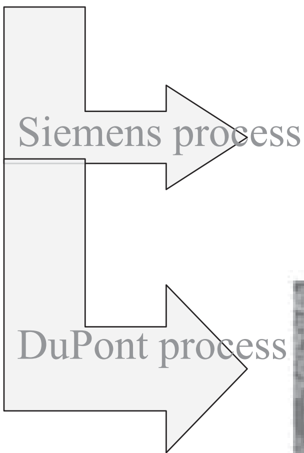


Can you suggest some idea to fabricate material X?

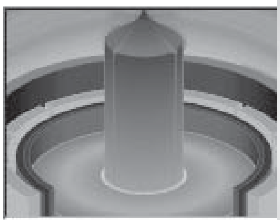
Can you estimate some characteristics of material X ?

Shape changes process

Silicon metal

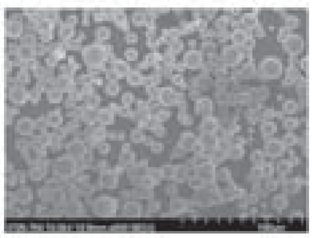


Poly-crystal

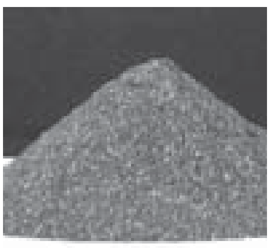


Crystal growth

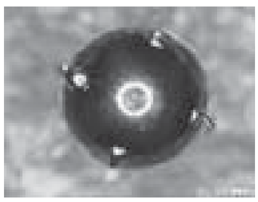
wafer



Nano-particle



powder

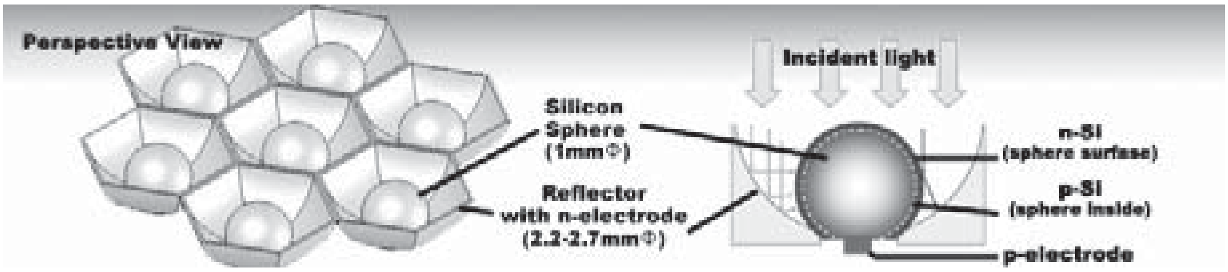


1mm sphere

Spherical silicon solar cells

Target：

0.7 $ ／W at 2020 year



National Project of Nano-risks

National Project of Nano-risk

The Cabinet office : Jyunko Nakanishi

JST : Masafumi Ata

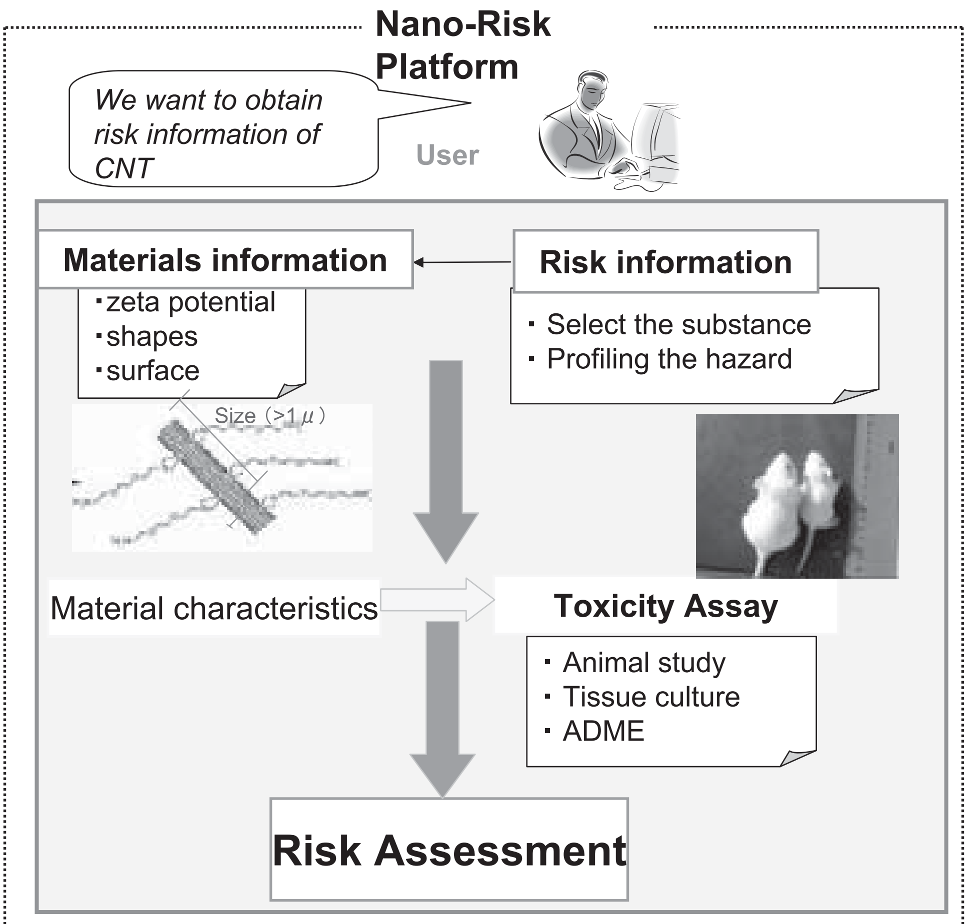
NIMS: *Materials characteristics*
Takeshi Inoshita
Masayoshi Yamazaki

⇔

U. of Tokyo *Risk assessment*
Yukio Yamaguchi
Yasuto matsui

⇔

AIST *Promotion of risk literacy to public*
Saori Ishizu
Mizuki Sekiya



How to promote a risk assessment on NANO?

powered by Information-Technology

Phase1: Select *the substance* having a potential hazard.

chemical substance
benzene, toluene, B[a]P･･･

NANO
CNT, C60, TiO_2･･･

Having many VARIETIES.

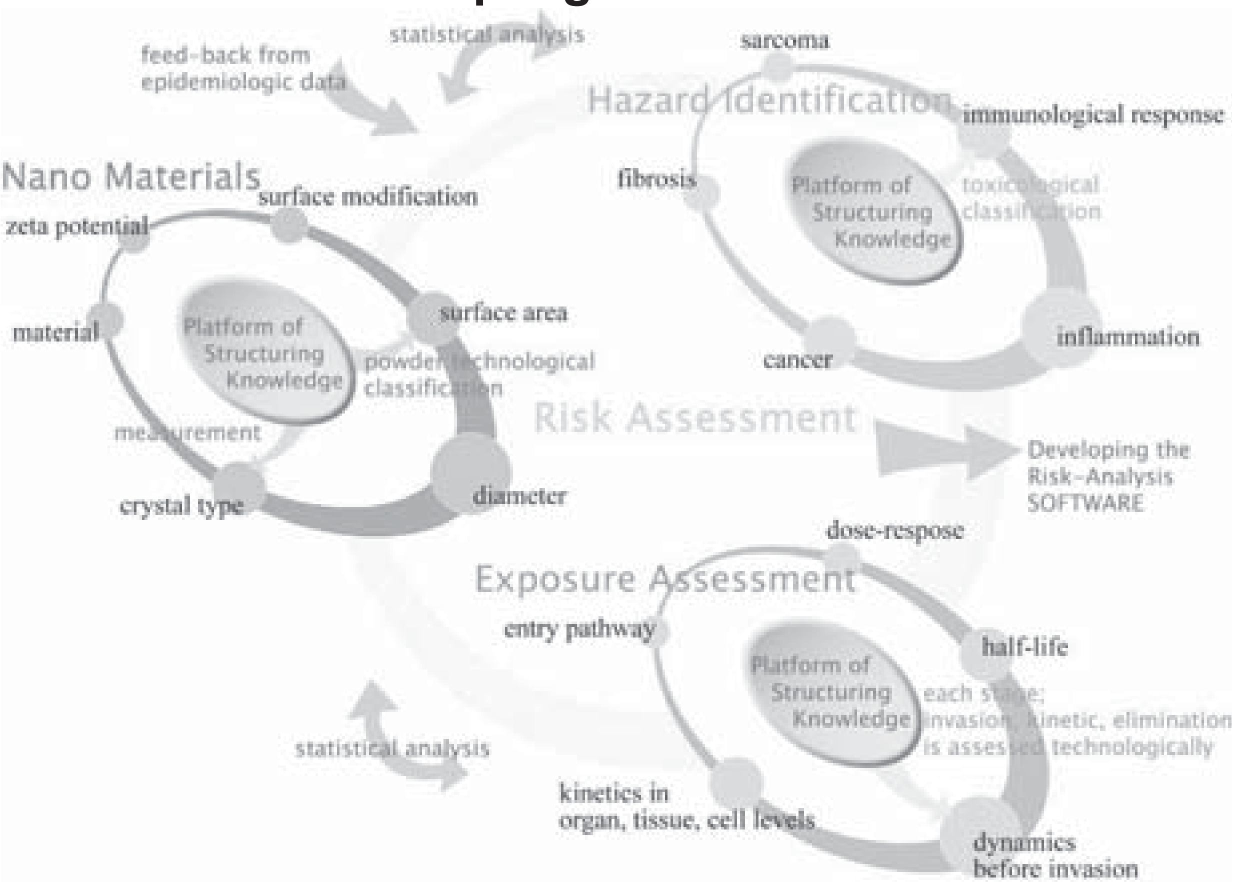
Phase2: Profiling *the hazard* on this substance by past researches.

TiO_2 → aspect ratio, diameter, surface area, material → ? → inflammation, asthma, cancer, neurotoxicity

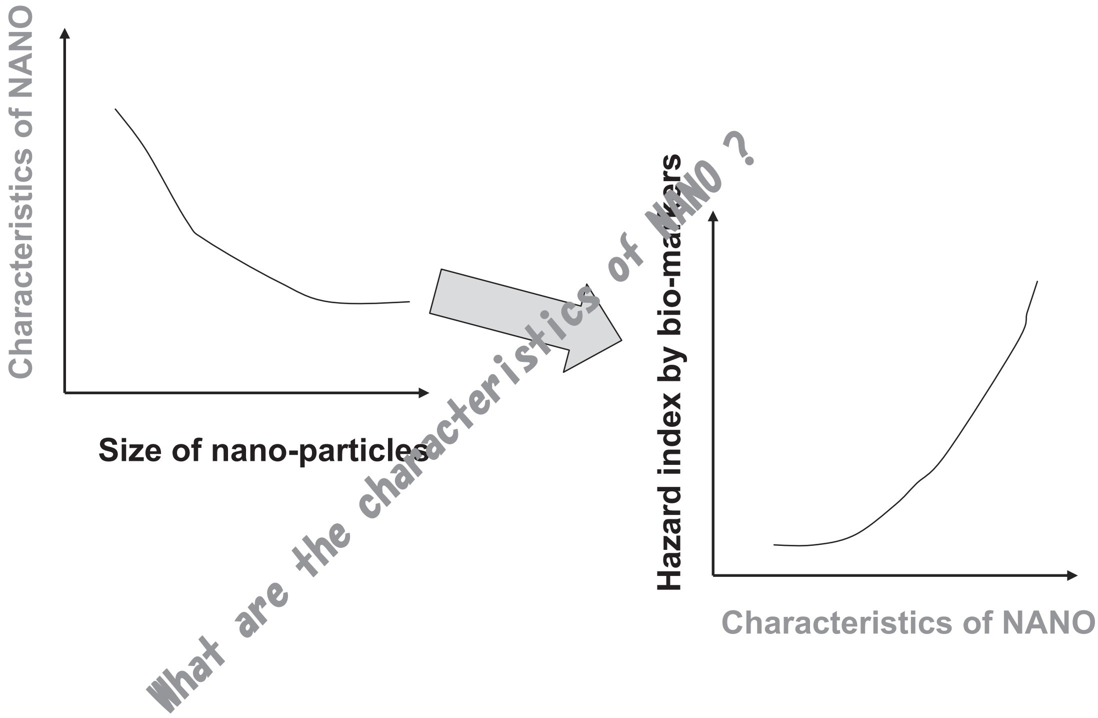
Phase3: Toxicity assay
#1 Animal studies
#2 Tissue culture
#3 ADME (Absorption, Dose, Metabolish, Excretion)

Phase4: Risk Assessment

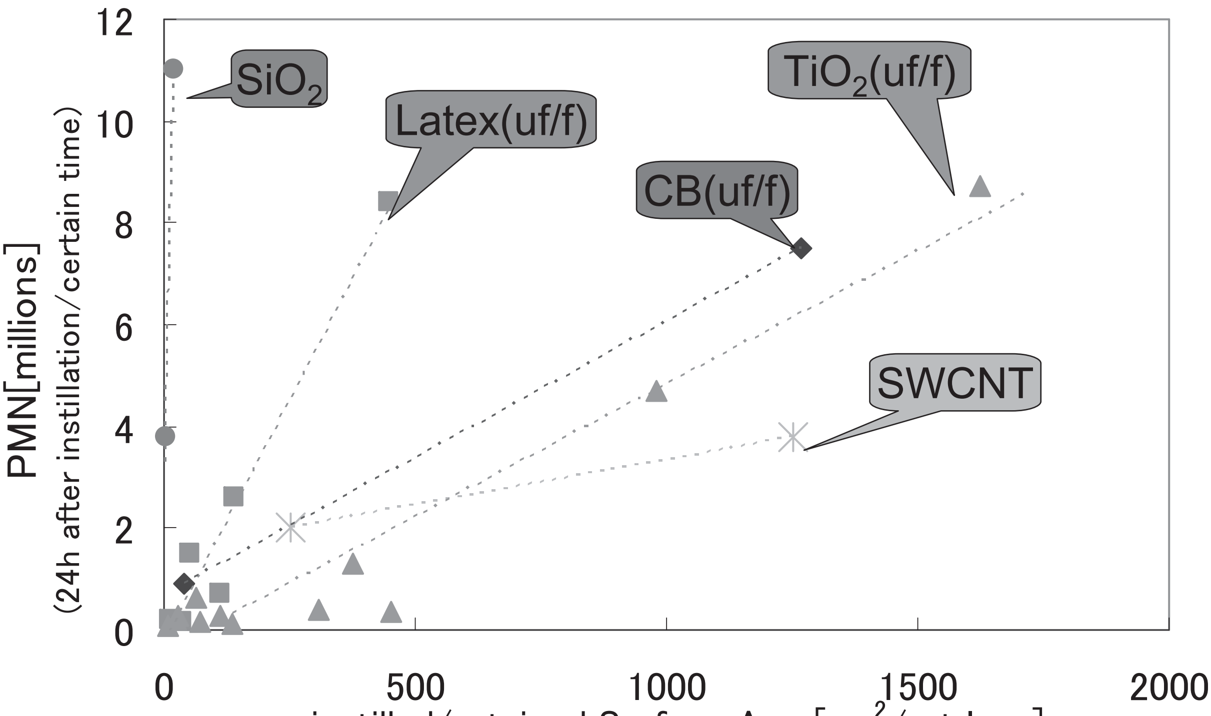
Our concept against the Nano-risk



Characteristics of NANO



The effect of surface area



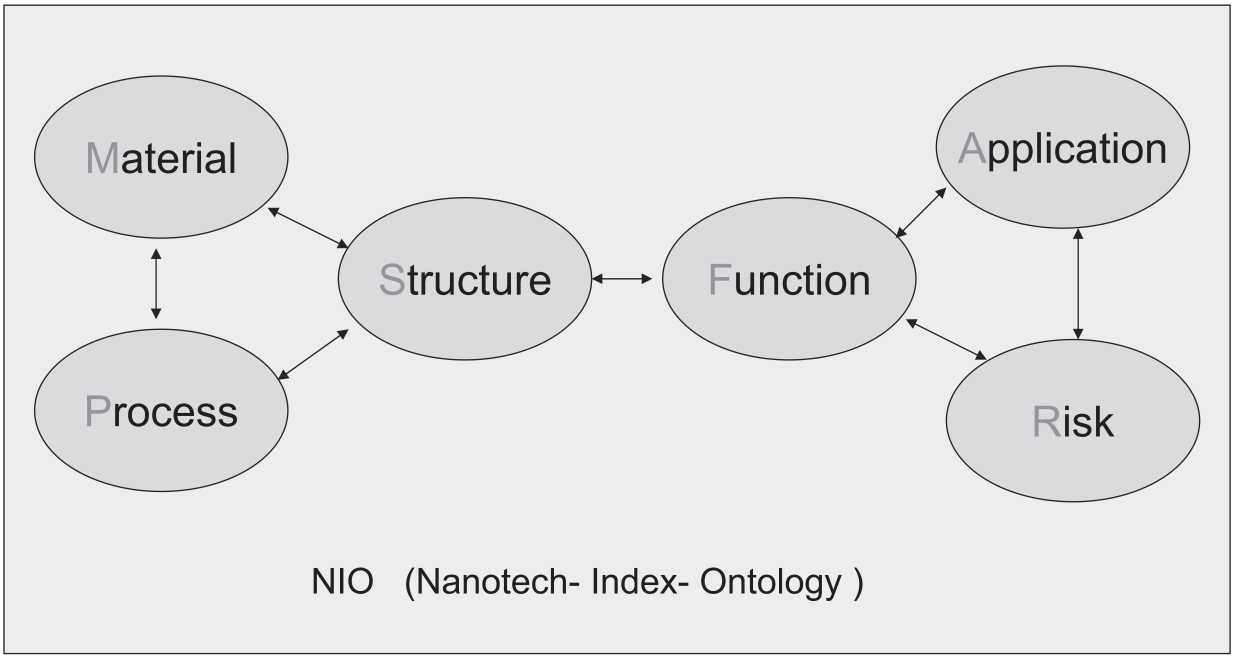
Donaldson, K. et al. (2000) Phil. Trans. R. Soc. Lond. A 358, 2741-2749
Oberdorster, G. et al. (1992) Am. J. Respir. Cell Mol. Biol. Vol. 6, 535-542
Warheit, D. B. et al. (2004). Toxicological Sciences 77, 117-125

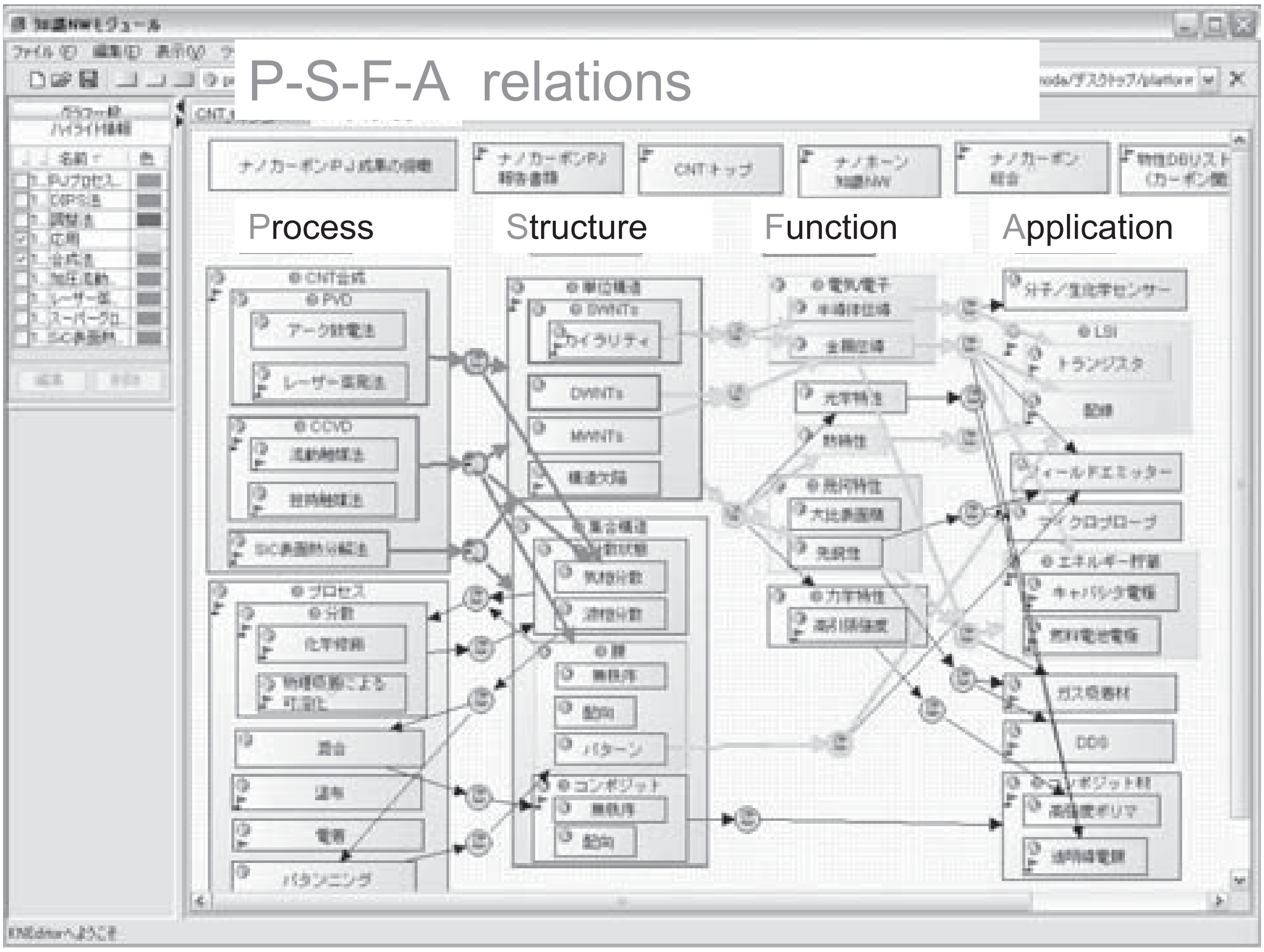
Isoelectric Point & Solubility of Metal Oxide

	Solubility[g/ℓ] at RT	Isoelectric Point (pH^0)	$\lvert pH^0-7.4 \rvert$	ionization tendency
SiO_2	1.2×10^{-1}	～2	5.4	−
ZnO	1.2×10^{-2}	～9	2.4	****
MgO	9.8×10^{-3}	～12	4.6	******
NiO	8.9×10^{-7}	～11	3.6	**
Fe_2O_3	3.6×10^{-8}	～8	0.6	***
ZrO_2	9.9×10^{-9}	～4	3.4	−
Al_2O_3	7.1×10^{-15}	～8.5	1.1	*****
TiO_2	2.2×10^{-25}	～6	1.4	−

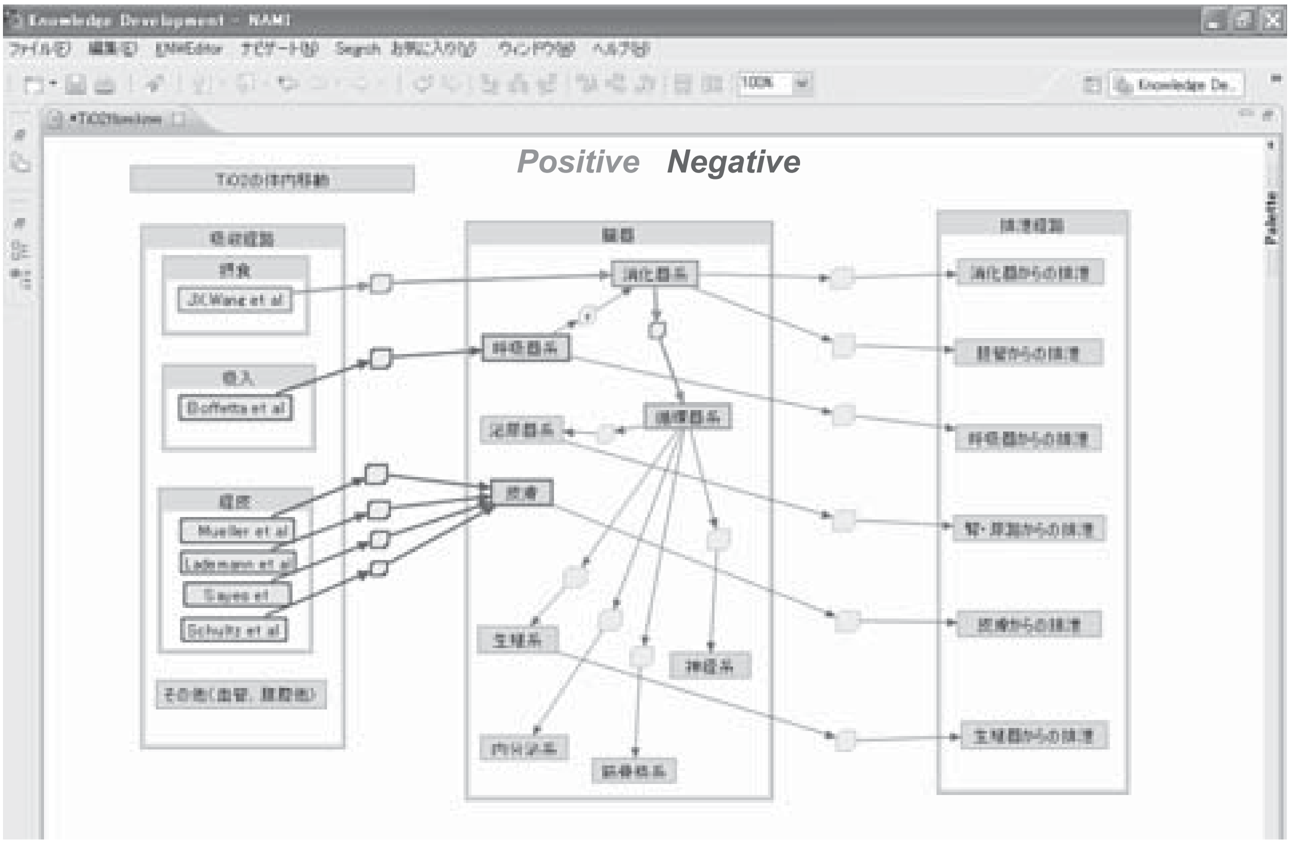
Engines to support NANO platform

MPSFA-R relationships

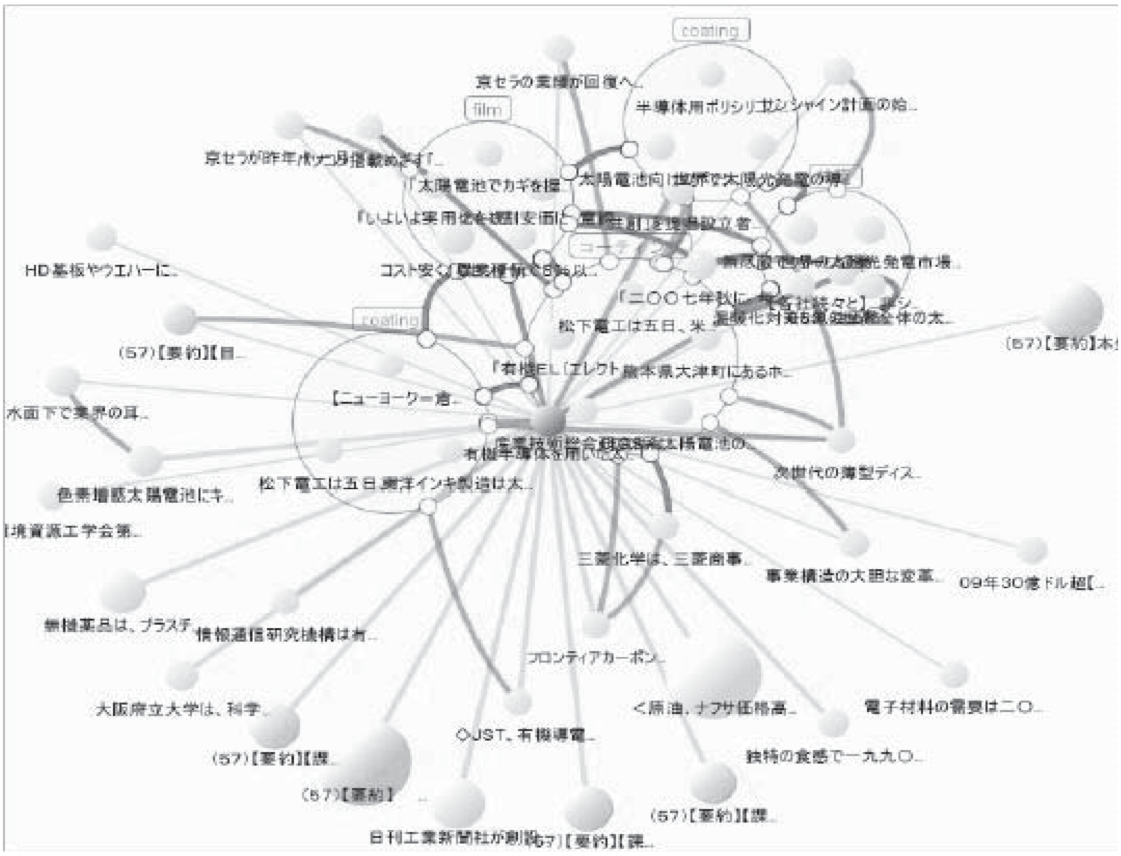




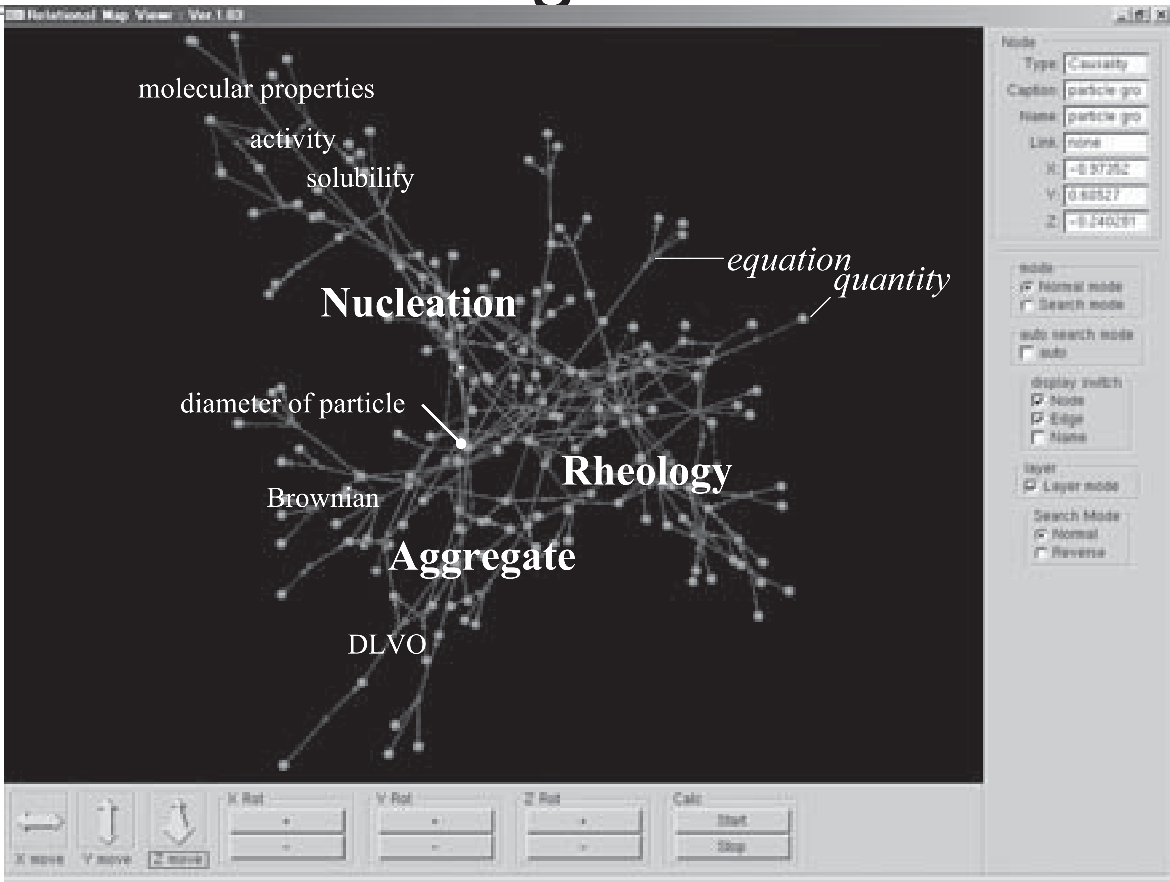
Trade-off Analysis of hazard data



Topic map & Researcher map

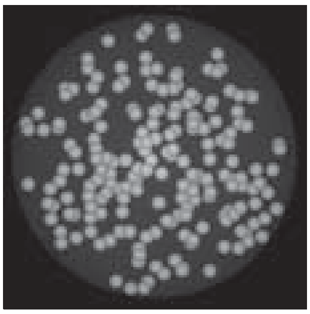


Knowledge Network

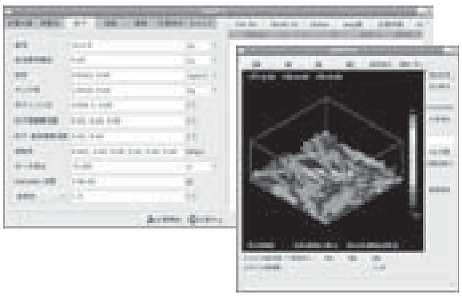


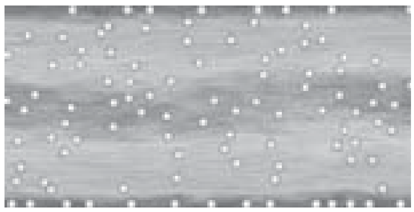
Aggregation simulator (SNAP)

Aggregation can be estimated from characteristics of NANO.

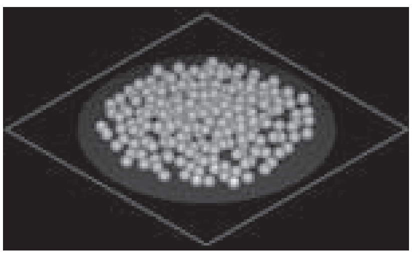


Droplet drying

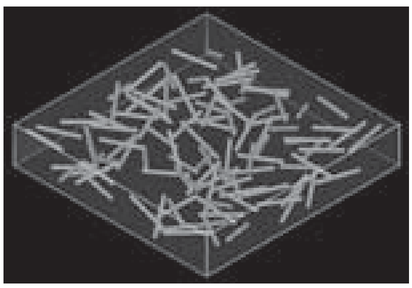




Fouling in a pipe



Droplet drying



Drying of rod particles

Conclusions

- Platform of nano-risks related to nano-materials can be built up in a year.

- Risk assessment can be established by physical, chemical and biological approaches.

NIST Databases for Inorganic-Materials Research

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*terrell.vanderah@nist.gov

Phase equilibrium data are used throughout the ceramics industry to understand and control the complex phenomena which increasingly underlie the production and performance of advanced materials. Phase diagrams serve as maps of the equilibrium chemical and structural behaviors exhibited by materials and provide critical starting information for the rational design of materials processing schemes, for quality assurance efforts, and for the optimization of the physical and chemical properties of advanced materials.

The *Phase Equilibria Diagrams* series [1], produced via a long-standing collaboration between NIST and the American Ceramic Society, provides written critical commentaries, evaluated graphical representations, bibliographic data, and analytical capabilities.

Fig.1: Since 1933, NIST scientists have collaborated with The American Ceramic Society (ACerS) to meet the need for reliable phase diagram data by jointly publishing a series of critically evaluated collections of phase equilibrium diagrams.

The published portion of the database now includes over 20,000 phase diagrams contained in 21 books and a CD-ROM [2]. Activities in the Data Center, located in the Ceramics Division at NIST, include continuous addition of new content to the database (about 1000 new entries per year), dissemination of the data in printed and digital formats, and development of scientific software to facilitate access to and use of the data. NIST experts provide continuous oversight of the scientific content of the database alongside phase equilibrium research activities.

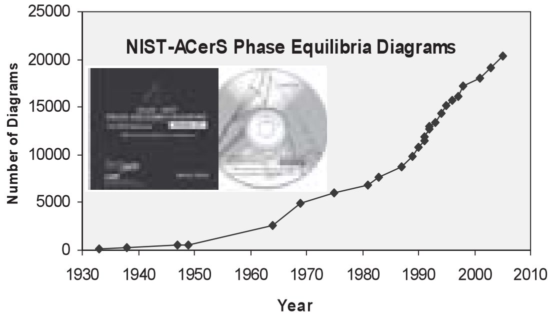

Fig.2: The Phase Equilibria Diagrams database currently grows by approximately 1000 new diagrams per year. The CD-ROM PC product includes all text and diagrams previously published in 21 hard-copy books.

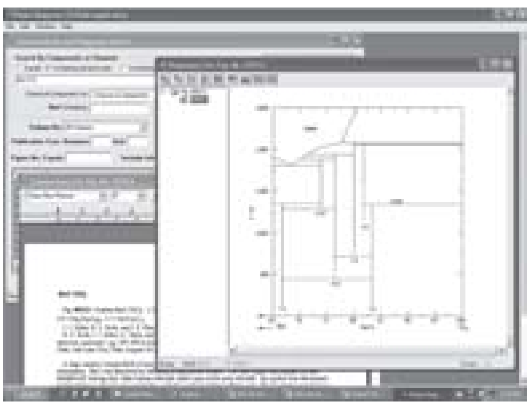

Fig.3: The CD-ROM database includes full commentary text in addition to diagram display. User features include high-quality printing and export capability, zoom-in with string-box selectivity, interconversion between mol% and wt%, overlay of diagrams, cursor position display in diagram units, reverse/rotate function for binaries and ternaries, and curve-follow.

Development of inorganic materials necessarily begins with the preparation and identification of product phase(s). An estimated 20,000 X-ray diffractometers and a comparable number of electron microscopes are used daily in materials research and development laboratories for this purpose. Crystalline compounds can be identified by their characteristic diffraction patterns using X-rays, neutrons, and/or electrons; however, this requires pattern-matching using crystal structure data already determined for all phases known to form in the chemical system of interest. Modern, automated diffraction instruments generate large amounts of diffraction data which frequently cannot be readily interpreted due to a paucity or lack of accurate crystal structure data. An additional barrier is a lack of data needed to establish processing-structure-property linkages.

Rapid, unambiguous identification of crystalline phases by diffraction requires comprehensive, accurate, and reliable crystal structure databases that can be quickly and easily searched. As different diffraction techniques and instruments generate data with different content, the databases need to be integrated easily into a wide variety of instrument platforms.

NIST develops and provides crystal structure information in the form of three standard reference databases (SRDs): SRD 3 (NIST Crystal Data); SRD 83 (NIST Metals Structural Database); and SRD 84 (FIZ/NIST Inorganic Crystal Structure Database, ICSD [3]). SRD 3, although limited to crystallographic unit cell parameters and phase composition, is the most comprehensive in terms of materials classes, covering inorganic and organic materials, with about 250,000 entries. SRD 83 contains crystallographic and atomic position information for about 60,000 metallic and intermetallic materials. SRD 84 contains crystallographic and atomic position information for about 100,000 inorganic materials. The databases are updated by NIST and its collaborators through critical evaluation of crystallographic data.

NIST produces the FIZ/NIST Inorganic Crystal Structure Database (ICSD, SRD 84), a comprehensive collection of data for inorganic crystalline materials, in collaboration with FIZ-Karlsruhe, Germany. Although the original definition of the ICSD specifically excluded metals and intermetallic crystalline materials, with NIST's recent delivery of SRD 83 content to collaborators in FIZ-Karlsruhe, the definition of the FIZ/NIST ICSD has been changed to cover all categories of non-organic materials including inorganics, metals, intermetallics and minerals. Further enhancements through continued data evaluation, transformation, standardization, and through database design are planned as SRD 83 is subsumed into the FIZ/NIST ICSD over the coming years. This accomplishment marks the beginning of a long-term plan to create and disseminate one comprehensive crystallographic database for all non-organic materials to benefit researchers worldwide.

NIST

FIZ KARLSRUHE

Fig.4: Collaboration between NIST and the Fachinformationszentrum Karlsruhe (FIZ) leads to the distribution of 2,000 to 10,000 new and revised inorganic crystal structures per year, released twice-yearly as updates to SRD 84 and offered as an internet- or PC-based product.

References

[1] Also known as NIST Standard Reference Database 31, and formerly named *Phase Diagrams for Ceramists*

[2] Phase Equilibria Diagrams Database v.3.1.0, NIST SRD 31 http://www.nist.gov/srd/nist31.htm, The American Ceramic Society, Westerville, OH

[3] FIZ/NIST Inorganic Crystal Structure Database; Release 2007/2 (Sept., 2007; 100,243 entries).

NIST Materials Databases for Inorganic Materials Research

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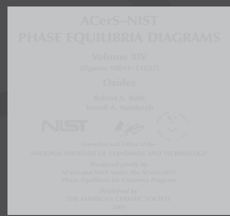
Outline

- **Phase Equilibria Diagrams Database**
  (Standard Reference Database - SRD 31)
- **Crystallographic Databases**
  (SRDs 3, 83, 84)
- **Other standards work in the NIST Ceramics Division**
- **Standards at NIST**

NIST -ACerS
Phase Equilibria Data Center

- **A database of critically evaluated ceramic phase equilibria**
- **Systems include:**
  - Oxides
  - Salts
  - Borides, carbides, and nitrides for structural ceramics
  - Semiconductor elements and compounds
  - High temperature superconductors
  - Electronic ceramics
- **Approximately 22,000 diagrams in 21 bound volumes**
- **Available in print or CD-ROM; > 55,000 print copies sold**





Phase Equilibria Diagrams Database
NIST SRD 31: http://www.nist.gov/srd/nist31.htm

- **Began in 1933 via NIST-ACerS collaboration**

A COMPILATION OF PHASE-RULE DIAGRAMS OF INTEREST TO THE CERAMIST AND SILICATE TECHNOLOGIST

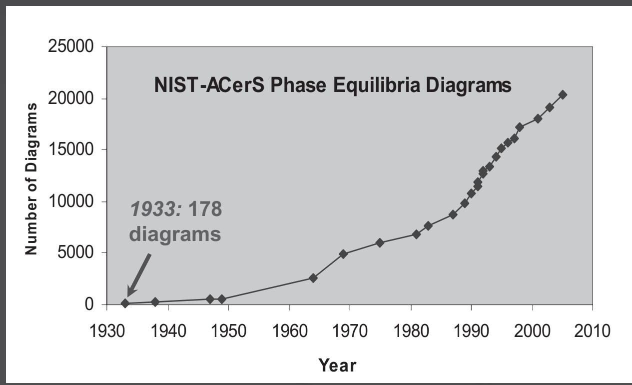
By F. P. Hall and Herbert Insley

Issued as the October, 1933, number of *The Journal of the American Ceramic Society*

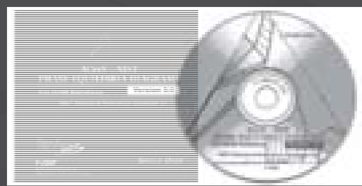
Phase Equilibria Diagrams Database

NIST SRD 31: http://www.nist.gov/srd/nist31.htm

- Began in 1933 via NIST-ACerS collaboration
- Continuous growth: ~1,000 diagrams per year



- Published data:
  - ~ 18,000 figures with ~22,000 diagrams
- Unpublished data:
  - ~ 25,000 entries with ~50,000 diagrams
  - sorted/searchable by chemical system
  - "INFO" file of ~6,000 literature references



contact: terrell.vanderah@nist.gov

Phase Equilibria Diagrams Database

NIST SRD 31: http://www.nist.gov/srd/nist31.htm

Data Center Process

1. Search original literature *(NIST)*
2. Identify, classify new entries *(NIST)*
3. Enter citation and chemistry into database *(NIST + ACerS)*
4. Select material to be evaluated *(NIST)*
5. Write critical evaluations/commentaries *(NIST Editors)*
6. Enter commentaries into database *(NIST + ACerS)*
7. Digitize evaluated diagrams *(ACerS (+ NIST))*
8. Edit commentaries and digitized diagrams *(NIST Editors)*
9. Publish content *(ACerS + NIST)*

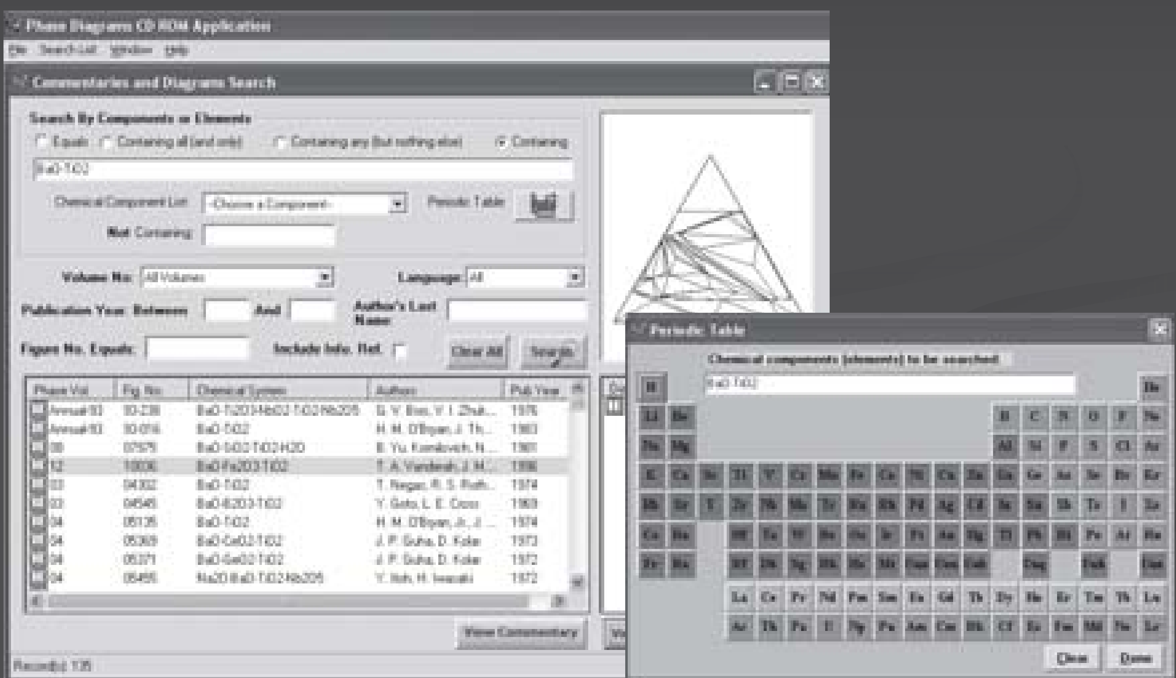
Phase Equilibria Diagrams Database

NIST SRD 31: http://www.nist.gov/srd/nist31.htm

Phase Equilibria Diagrams Database

NIST SRD 31: http://www.nist.gov/srd/nist31.htm

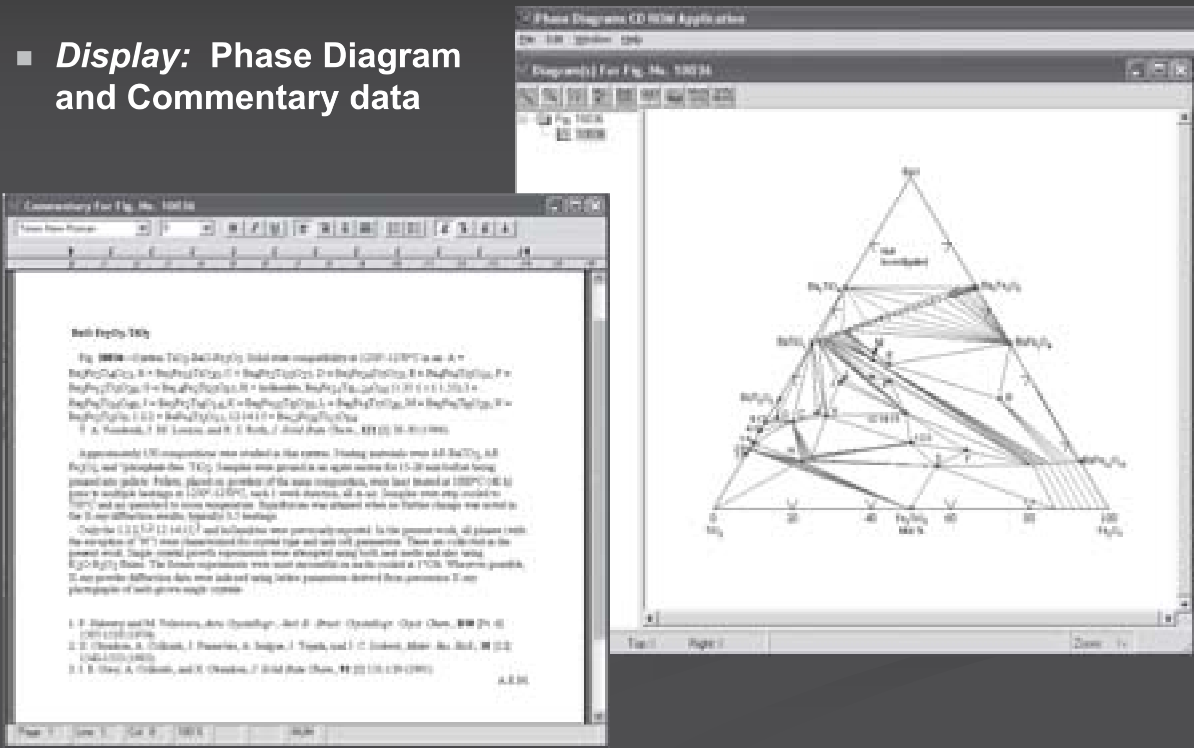
- ***Search interface:*** **by reference, element, component, figure no., volume**



Phase Equilibria Diagrams Database

NIST SRD 31: http://www.nist.gov/srd/nist31.htm

- ***Display:*** **Phase Diagram and Commentary data**

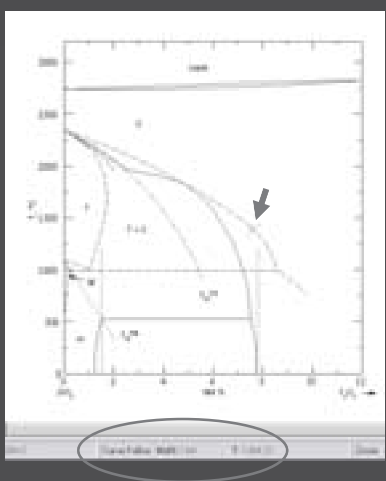


Phase Equilibria Diagrams Database

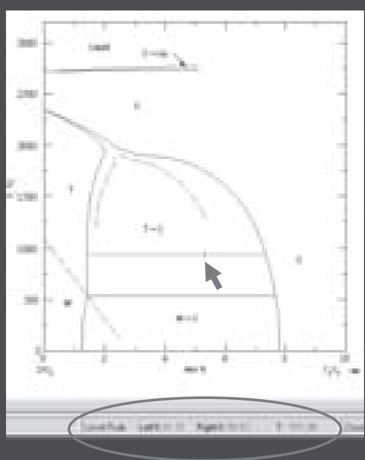
NIST SRD 31: http://www.nist.gov/srd/nist31.htm

- **Built-in functions allow user to track coordinates, zoom, convert mol%⇔wt%, use level rule, overlay diagrams, rotate ternaries, etc.**

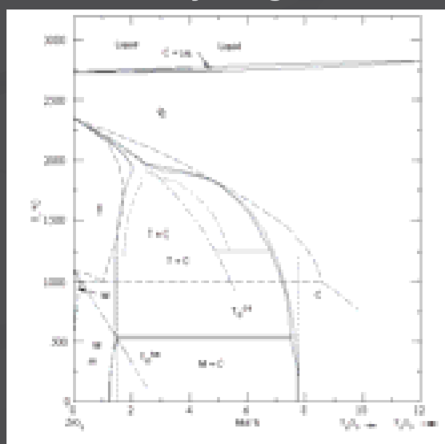
Curve Follow



Level Rule



Overlay Diagrams



Use of Phase Equilibria Diagrams

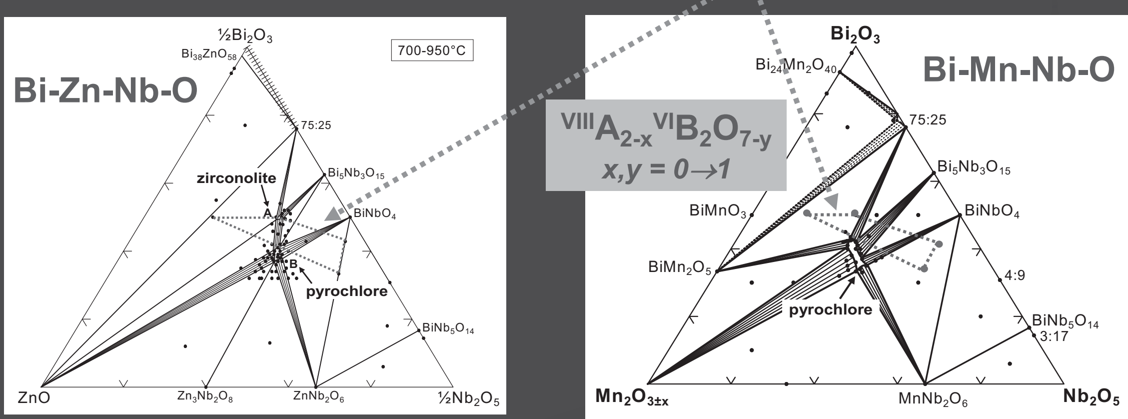
- **Phase equilibrium diagrams delineate the most fundamental properties of materials:** ***the conditions (temperature, pressure, composition) under which pure compounds and their mixtures are thermodynamically stable.***
- **Reliable data therefore provide <u>essential thermochemical guidance</u> for the technical exploitation of materials.**

examples…

Example: Use of Phase Equilibria Diagrams…

Pyrochlore-type ceramics $Bi_2(M,Nb)_2O_7$, M = metal

- **Of interest for electronic applications such as embedded dielectric elements** *(capacitors, filters, etc.)*
- **Phase equilibrium studies of a number of Bi-M-Nb-O systems revealed that the pyrochlores did not form where they "should", according to traditional crystal-chemical "rules"**



Bi^{3+} much larger than M and Nb^{5+} $\rightarrow$ different structural site

- **The phase equilibria results clearly indicated that the pyrochlore $A_2B_2O_7$ phase was forming at "B-cation-rich" stoichiometries, i.e. $A_{2-x}B_xB_2O_7$.**
- **Coupled with detailed structural studies, these results revealed a "new" crystal-chemical principle for this class of pyrochlore ceramics: <u>Up to ~25% of the larger A-cation sites can be occupied by smaller B-type cations</u>, which are crystal-chemically accommodated by displacive disorder.**

→ Many new pyrochlores can now be deliberately synthesized at new stoichiometries

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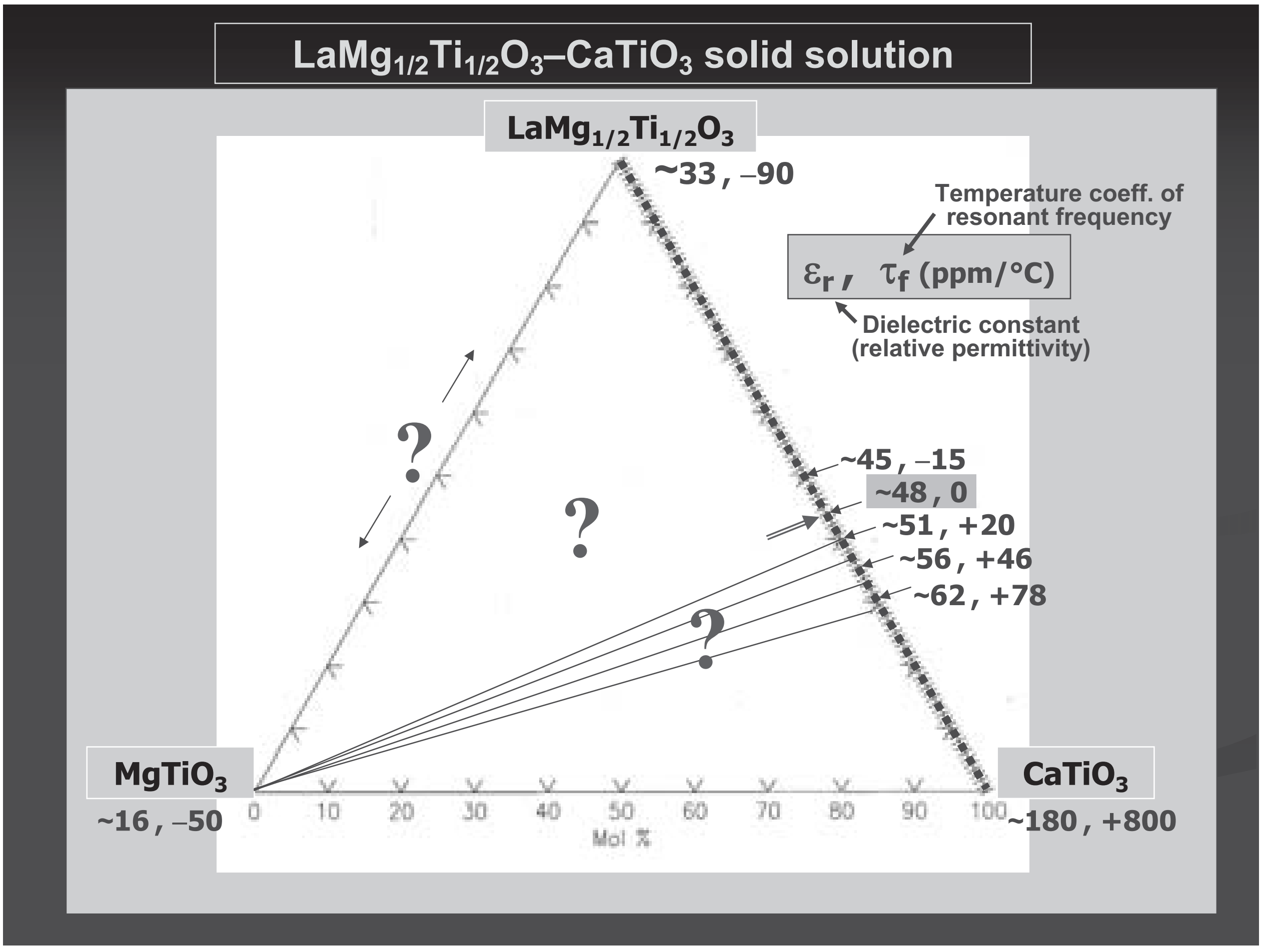
- **Eur. J. Inorg. Chem. 14, 2895-2901 (2005).**
- **J. Solid State Chem. 179(11), 3467-3477 (2006).**
- **J. Solid State Chem. 179(12), 3900-3910 (2006).**
- **Eur. J. Inorg. Chem. 23, 4908-4914 (2006).**

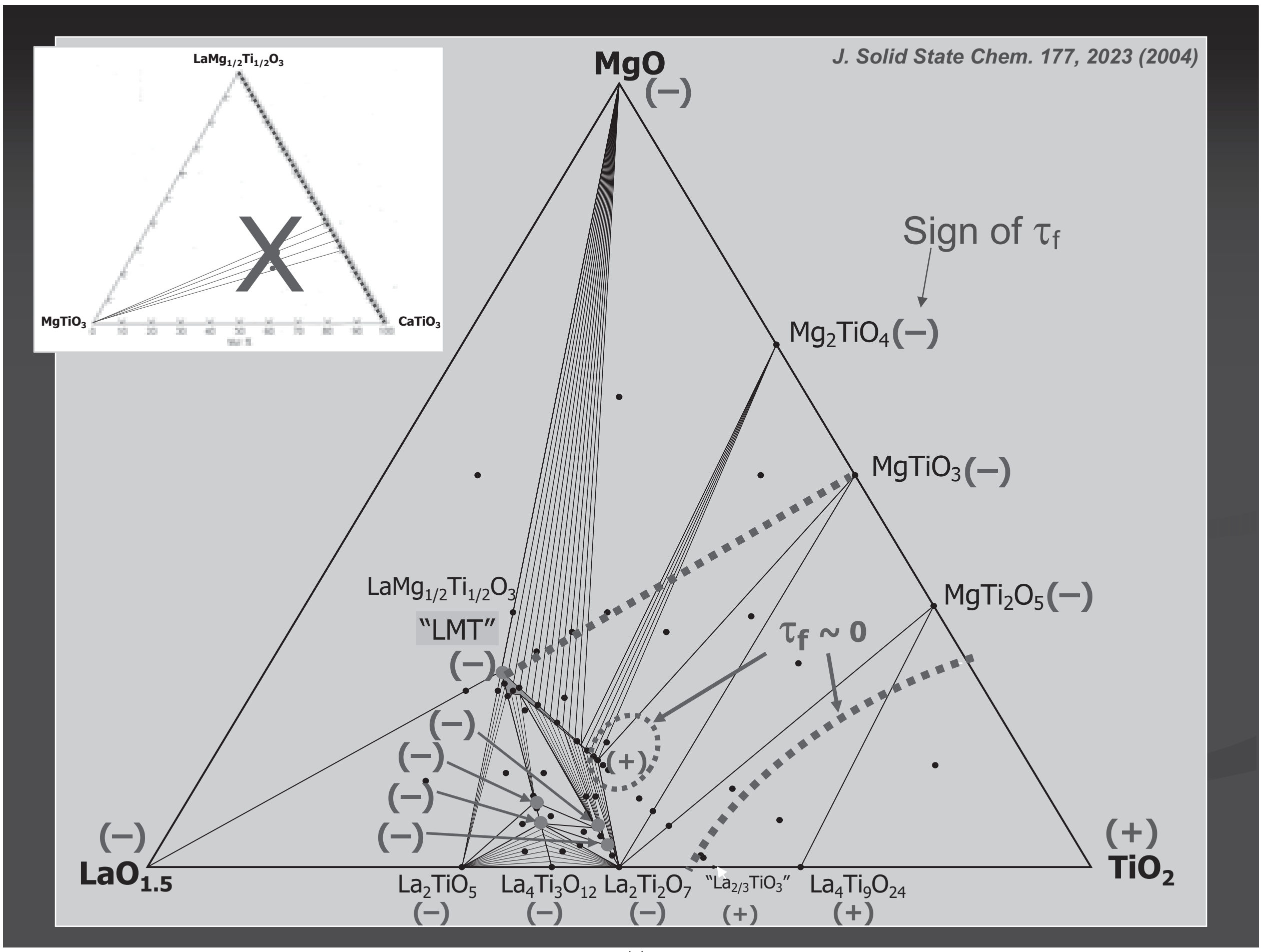
Rational Processing

- **Reliable phase equilibrium diagrams are particularly useful when the exploitable properties are additive.**
- **Example: microwave dielectric ceramics**

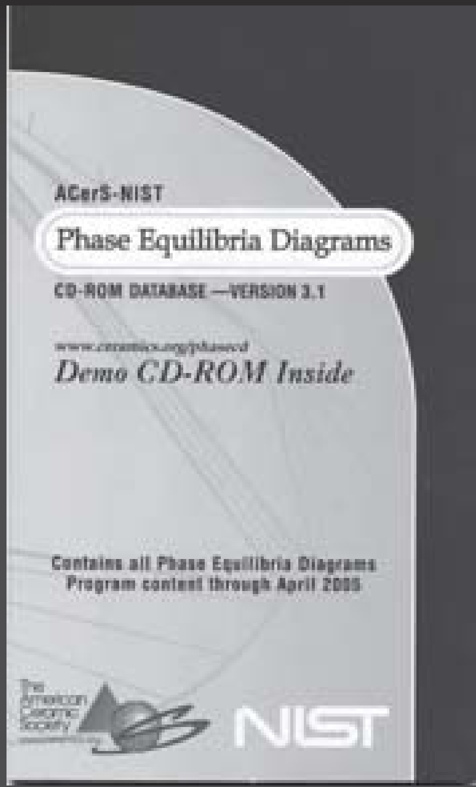
$44LaMg_{1/2}Ti_{1/2}O_3$–$56CaTiO_3$ solid solution

- ***of interest for resonators/filters***
- ***dielectric constant ~48, temp. coeff.$_f$ ~0***
- ***→ need to improve dielectric loss***


LaMg$_{1/2}$Ti$_{1/2}$O$_3$–CaTiO$_3$ solid solution
LaMg$_{1/2}$Ti$_{1/2}$O$_3$
~33 , –90
Temperature coeff. of resonant frequency
ε_r , τ_f (ppm/°C)
Dielectric constant (relative permittivity)
?
?
?
~45 , –15
~48 , 0
~51 , +20
~56 , +46
~62 , +78
MgTiO$_3$
~16 , –50
CaTiO$_3$
~180 , +800
0 10 20 30 40 50 60 70 80 90 100
Mol %


J. Solid State Chem. 177, 2023 (2004)
LaMg$_{1/2}$Ti$_{1/2}$O$_3$
X
MgTiO$_3$
CaTiO$_3$
MgO (–)
Sign of τ_f
Mg$_2$TiO$_4$ (–)
MgTiO$_3$ (–)
MgTi$_2$O$_5$ (–)
LaMg$_{1/2}$Ti$_{1/2}$O$_3$
"LMT"
(–)
τ_f ~ 0
(–)
(–)
(–)
(–)
(+)
(–) LaO$_{1.5}$
(+) TiO$_2$
La$_2$TiO$_5$ (–)
La$_4$Ti$_3$O$_{12}$ (–)
La$_2$Ti$_2$O$_7$ (–)
"La$_{2/3}$TiO$_3$" (+)
La$_4$Ti$_9$O$_{24}$ (+)

- Demo CD available from ACerS
  http://www.ceramics.org



Crystallographic Databases and Applications in Materials Research

Vicky Lynn Karen and Xiang Li

contact: vicky.karen@nist.gov

NIST Crystallographic Databases

- NIST Standard Reference Databases:
  - SRD 3: NIST Crystal Data (~237,000 entries)
    - Inorganic and organic crystalline materials
    - Crystallographic information without atomic coordinates
  - SRD 83: NIST Structural Database (~60,000 entries)
    - Metals and inter-metallics
    - Atomic coordinates and structure types
  - SRD 84: FIZ/NIST Inorganic Crystal Structure Database (ICSD, ~ 100,000 entries)
    - Inorganic materials
    - Refined structure information

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…NIST Crystallographic Databases

Non-organic = inorganic + metals

Full Structure Information:

- ICSD *(SRD 84)*
- NIST Structural Database *(Metals, SRD 83)*

(combined ~ 160,000 entries)

Phase Identification

- NIST Crystal Data

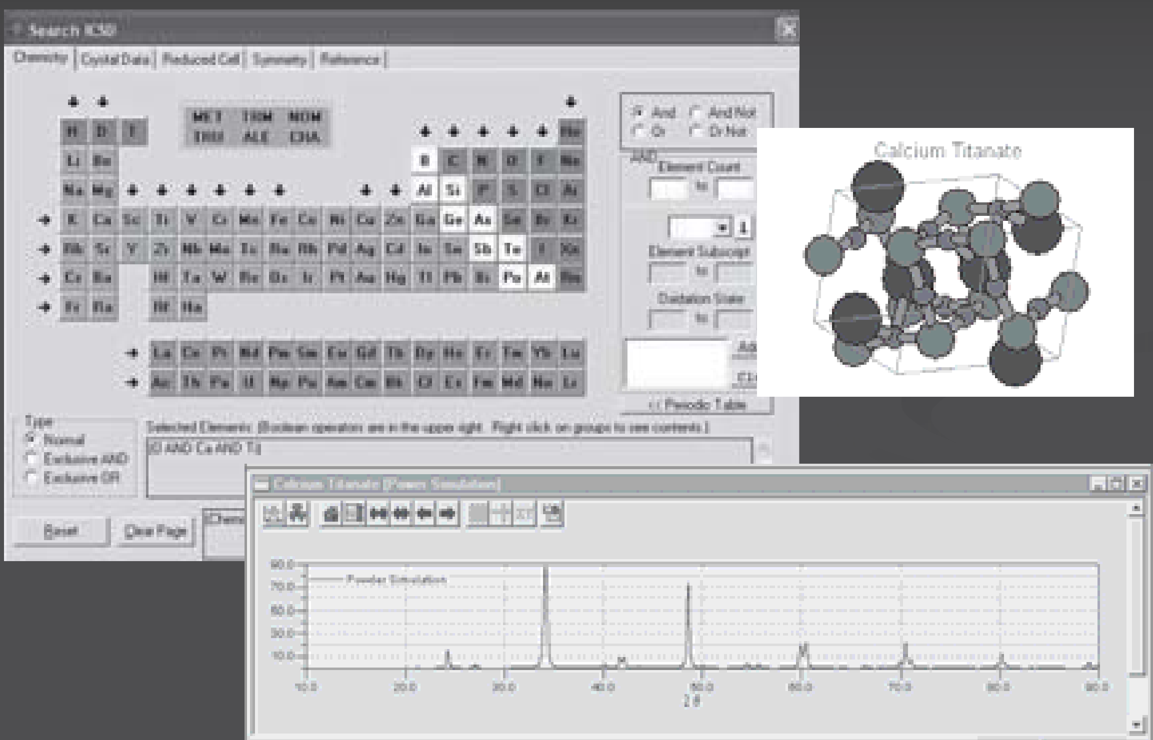
(~ 237,000 entries)

FIZ-NIST Inorganic Crystal Structure Database
(ICSD)

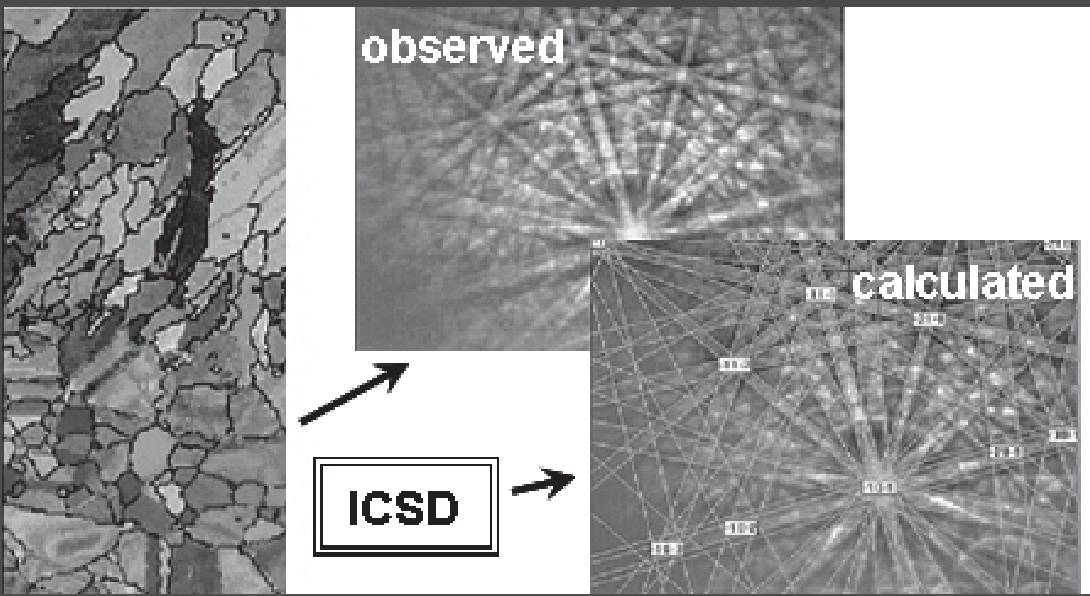
- ICSD is a collection of crystal-structure data entries for non-organic compounds including inorganics, ceramics, minerals, pure elements, metals, and intermetallics.
- Data items added by experts or generated by computer programs include Wyckoff sequence, Pearson symbol, molecular formula and weight, calculated density, chemical valence, "ANX" formula, minimum interatomic distances, reduced and standard cells, mineral groups and names.
- The entries in the database are characterized by and can be retrieved by chemical, crystallographic, computational, and textual searches.

contact: vicky.karen@nist.gov

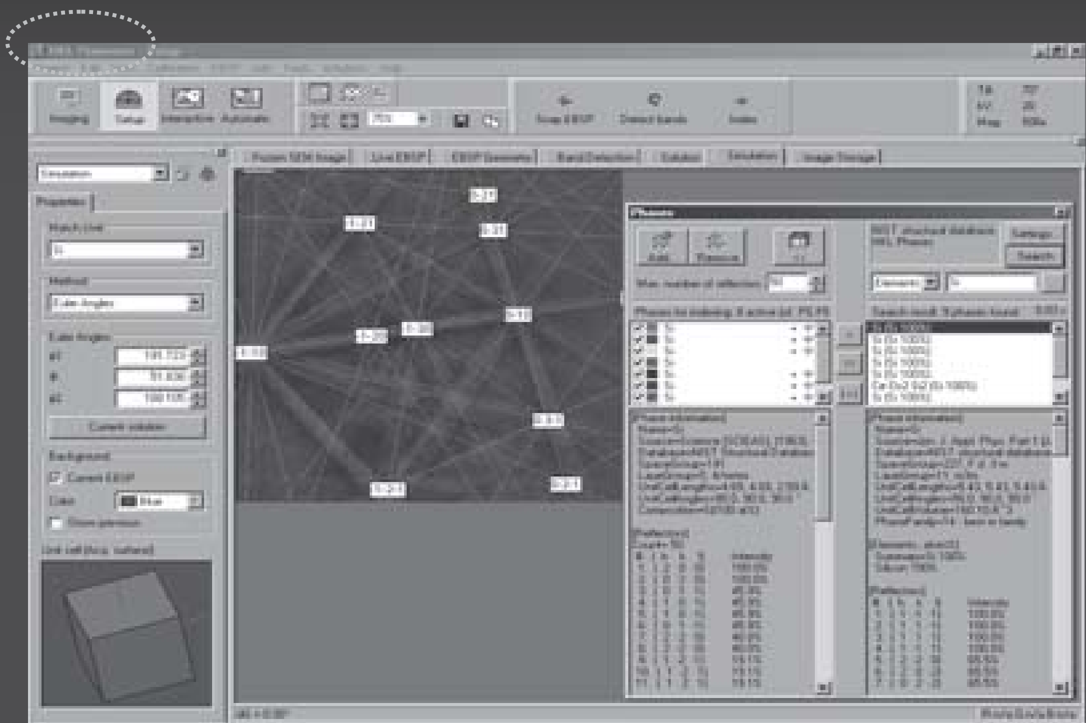
Database Applications



Phase Identification by Electron Diffraction



Phase Identification by Electron Diffraction



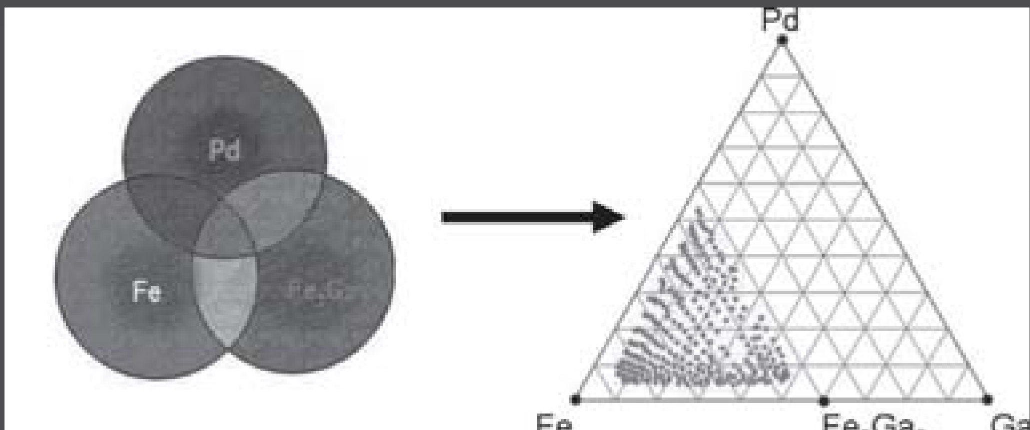
Applications in Materials Research

- Crystallographic databases facilitate rapid phase identification.
  - Known chemical phases can quickly be searched.
  - Diffraction peak positions and intensities can be calculated from the database entries.
  - Calculated patterns can be compared with experimental patterns for phase identification.

Combinatorial Library:
Rapid Phase Identification

- Combinatorial materials library from thin-film composition spread

(Ichiro Takeuchi, University of Maryland)

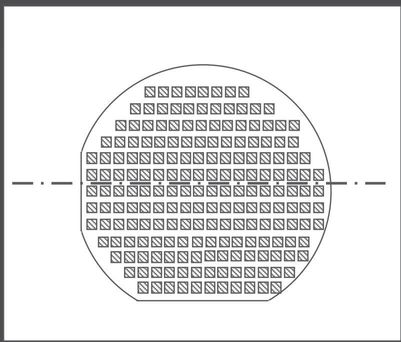


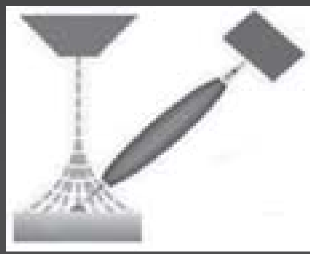
Schematic profile of co-sputtered Fe, Pd, and Ga

- C. J. Long, et al., Rev. Scientific Instruments 78, 072217 (2007)

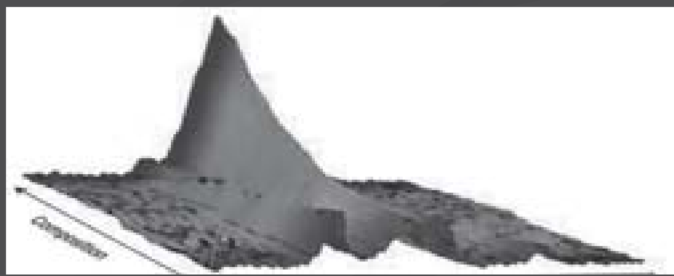
Combinatorial Library:

Rapid Phase Identification





WDS → Composition Determination

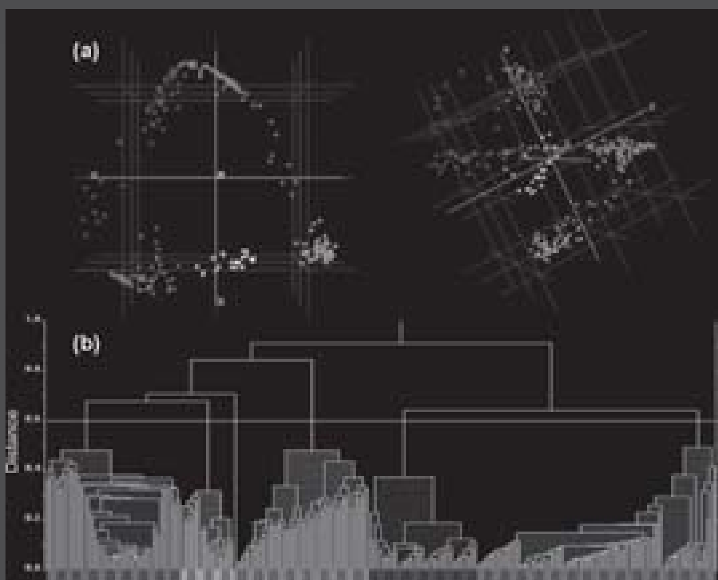


XRD → Phase Identification

Combinatorial Library:

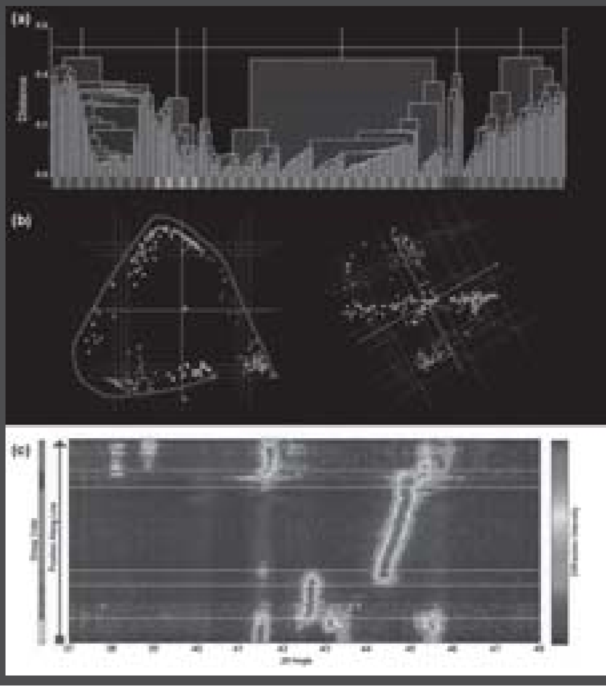
Rapid Phase Identification

- Statistical-analysis tools are applied to group the observed diffraction patterns according to their similarities.



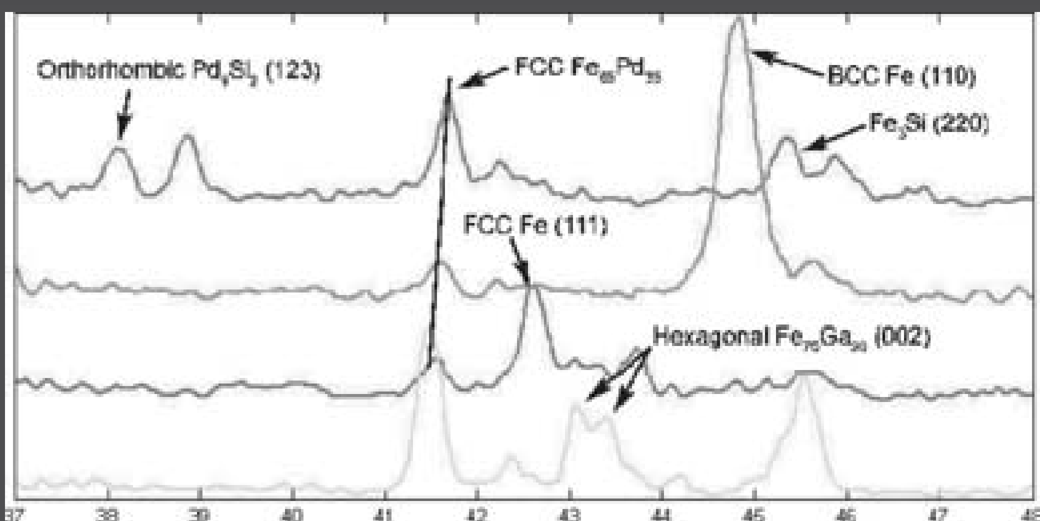
Combinatorial Library:
Rapid Phase Identification

- **The grouping results are validated.**



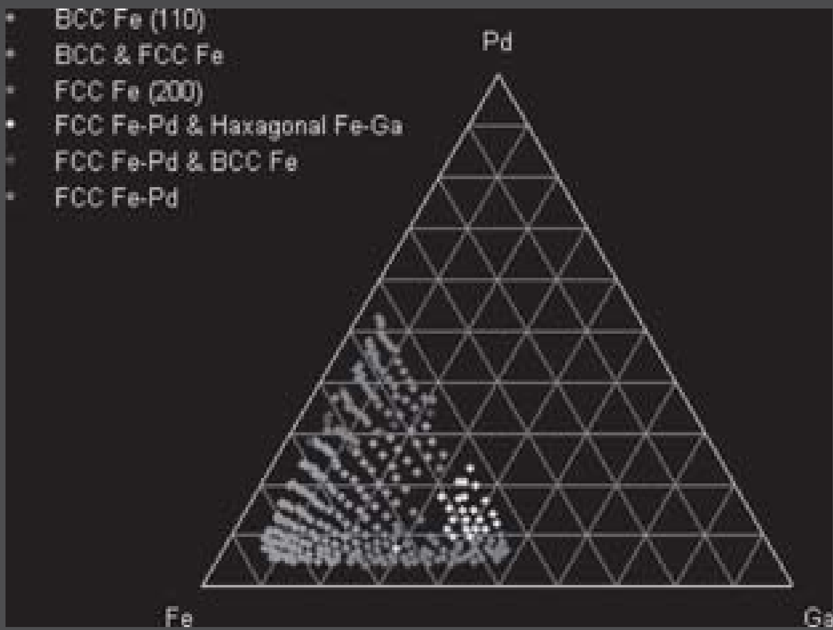
Combinatorial Library:
Rapid Phase Identification

- **Match the obtained groups of observed diffraction patterns with the peak positions and intensities calculated from the database search results.**



Combinatorial Library:
Rapid Phase Identification

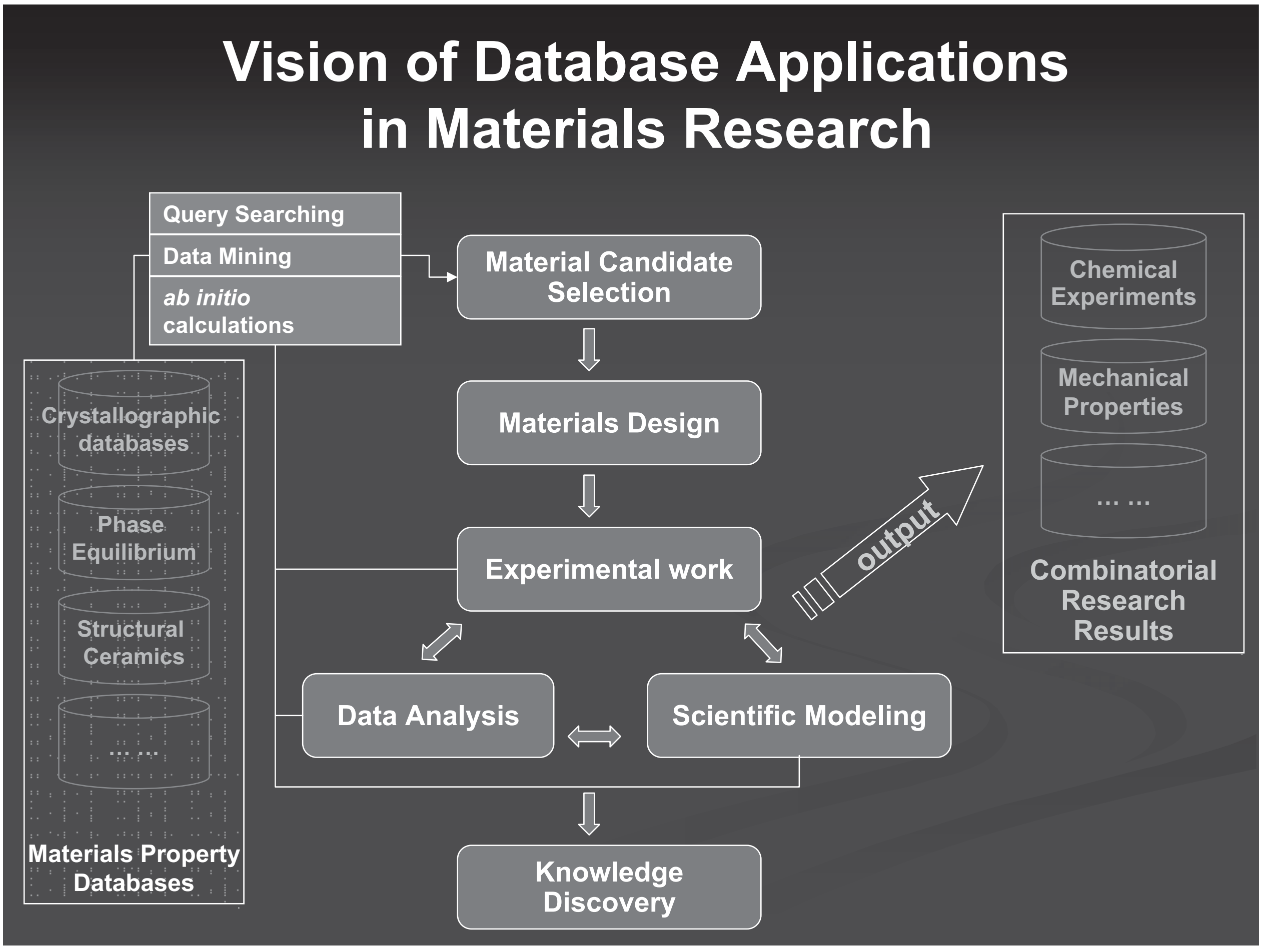
- **Phase diagram for this combinatorial library is obtained.**

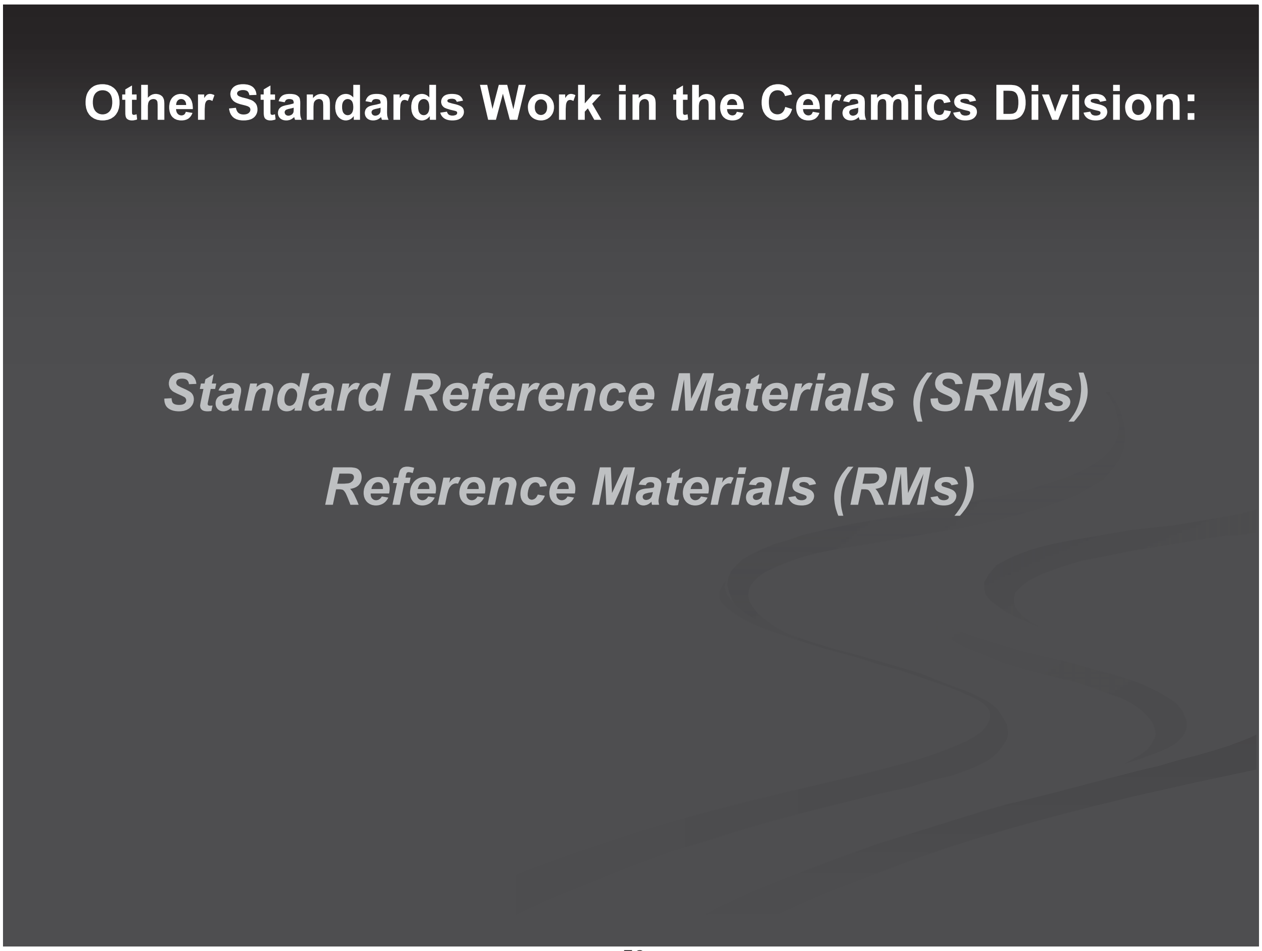


Applications in Materials Research

- **What can we do with the Crystallographic Databases?**

- ***Provide initial guidance in the design stage***
  - **Select materials based on known chemical-structural-symmetrical criteria**
  - **Input for *ab initio* calculations of properties**
  - **Data mining and other methods for locating potential candidates**
- ***Rapid phase identification in the experimental stage***
  - **Lattice matching**
  - **Powder diffraction fingerprinting**
  - **Lattice-fringe fingerprinting**
  - **High-throughput essential for combinatorial approach**
- ***Input-data for scientific simulations; interfacing with other computational tools for data analysis and theory development***


Vision of Database Applications
in Materials Research
Query Searching
Data Mining
ab initio calculations
Material Candidate Selection
Materials Design
Experimental work
Data Analysis
Scientific Modeling
Knowledge Discovery
output
Crystallographic databases
Phase Equilibrium
Structural Ceramics
… …
Materials Property Databases
Chemical Experiments
Mechanical Properties
… …
Combinatorial Research Results


Other Standards Work in the Ceramics Division:
Standard Reference Materials (SRMs)
Reference Materials (RMs)

Particle SRMs and RMs

Currently available:

SRM or RM	Material	Nominal Particle Diameter or PSD
1021	glass beads	2 µm to 12 µm
1003c	glass beads	10 µm to 60 µm
1004b	glass beads	40 µm to 150 µm
1017b	glass beads	100 µm to 400 µm
1018b	glass beads	220 µm to 750 µm
1019b	glass beads	750 µm to 2450 µm
1978	zirconium oxide	0.33 µm to 2.19 µm
1982	zirconium oxide	10 µm to 150 µm
659	silicon nitride	0.2 µm to 10 µm
1980	a-FeO·OH	60 nm x 20 nm
1963a	polystyrene	100 nm
1964	polystyrene	60 nm
8011	gold nanoparticles	10 nm
8012	gold nanoparticles	30 nm
8013	gold nanoparticles	60 nm

Just released:

- *New gold nanoparticle RMs 8011, 8012, 8013*
- *10 nm, 30 nm, 60 nm particle diameters*
- *Developed in collaboration with U.S. Nanotechnology Characterization Laboratory; Food and Drug Administration*

contact: vince.hackley@nist.gov

SRMs for X-ray Diffraction

Products

SRM	Material	Type
640c	Silicon Powder	Line Position & Line Profile
675	Mica Powder	Line Position, Low 2θ
2000	Silicon (100) Wafer with Si/SiGe epilayer	High-resolution Line Position
660a	LaB_6 Powder	Line Position & Line Profile
1979	CeO_2 & ZnO	Line Profile
1976a	Sintered Alumina Plate	Instrument Response
676a	Alumina (corundum) Powder	Quantitative Analysis
674b	Powder Set: ZnO, TiO_2, CeO_2, Cr_2O_3	Quantitative Analysis
1878a	Respirable Quartz Powder	Quantitative Analysis
1879a	Respirable Cristobalite Powder	Quantitative Analysis
656	Silicon Nitride: α & β powders	Quantitative Analysis

Just released:

- NIST SRM 2000
- High Resolution XRD (HRXRD)
- → femtometer accuracy in lattice parameter determination
- → SI-traceable HRXRD measurements (e.g., strained Si-on-insulator R&D/manufacturing)

SRM 2000 Si (220) *d*-spacing

Quantity	Reference value	Expanded Uncertainty
d_{SRM}	0.1920161 nm	0.87 fm

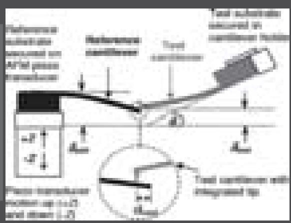
contacts: james.cline@nist.gov
donald.windover@nist.gov

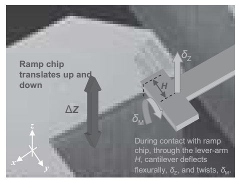
Standards for Scanned Probe Microscopy

Products: Cantilever standards for AFM

- **Calibrated Reference Cantilever Array** – *available 2008*
  - Cantilever array with SI-traceable stiffness for calibrating AFM cantilevers
  - Cantilevers microfabricated from silicon-on-insulator wafers
  - Cantilever dimensions: 50 μm wide x 1.5 μm thick x (300 to 600) μm long
  - Estimated accuracy and precision in stiffness measurement of 2% to 3%

- **"Hammerhead" Cantilever for AFM Lateral Force (friction) Measurement** – *in development*
  - Lateral force cantilever enables precise nanoscale friction measurement capabilities for AFM
  - The lateral lever arms of the Hammerhead allow the optical detector of the AFM instrument to be calibrated to known lateral forces applied to the cantilever

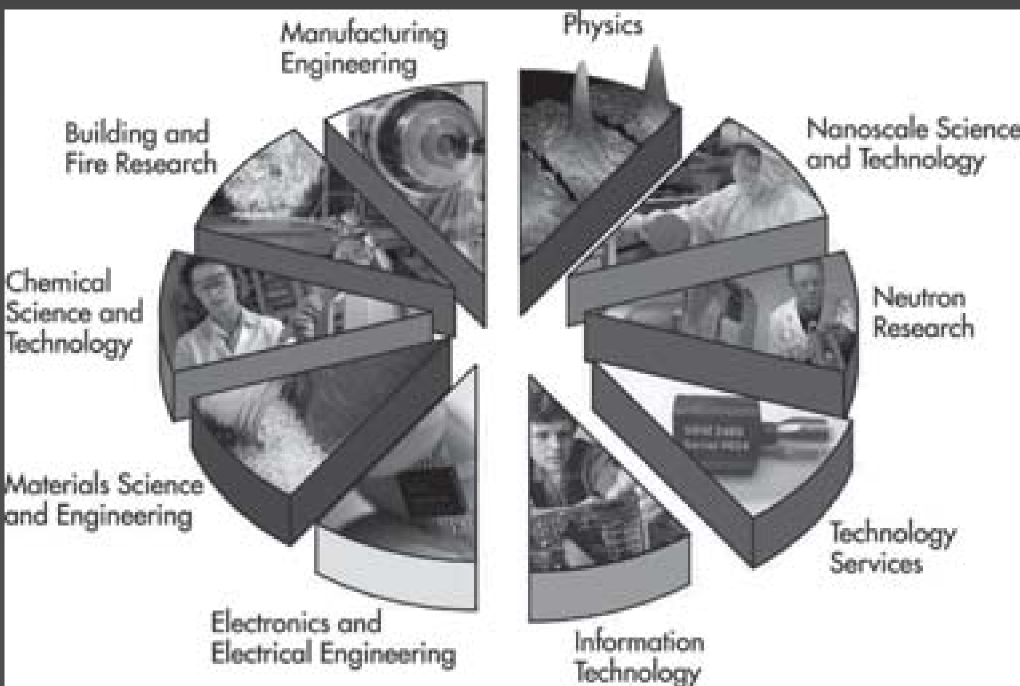




contact: richard.gates@nist.gov

The NIST Laboratories:

Standards Activities



NIST Measurement Services

- **Calibrations**
  - Service in NIST technical lab
  - Customer sends instrument to NIST
- **Standard Reference Materials (SRMs)**
  - Physical artifacts with certified physical or chemical properties
- **Standard Reference Data (SRD)**
  - Evaluated numeric data on physical or chemical properties
  - Scientific algorithms on behavior of systems

contact: robert.watters@nist.gov

- **Calibrations**
  - 15,900 tests/year – categories →
    - Dimensional
    - Electromagnetic
    - Ionizing Radiation
    - Mechanical
    - Optical Radiation
    - Thermodynamic
    - Time and Frequency
  - >600 customers
- **Standard Reference Data**
  - 1,800 customers
  - 55 PC products available
  - 54 Online SRD systems out of 78 total NIST systems
  - 6,000 units sold/year
- **Standard Reference Materials**
  - Prepared by 20 Divisions in 6 NIST Laboratories
  - 1,285 products available
  - 2,800 customers
  - 33,000 units sold/year
  - 3 major categories
    - chemical composition
    - physical properties
    - engineering properties
  - Fee supported: includes portion for developing new reference materials and stability testing

contact: robert.watters@nist.gov

Technical Areas for NIST SRD

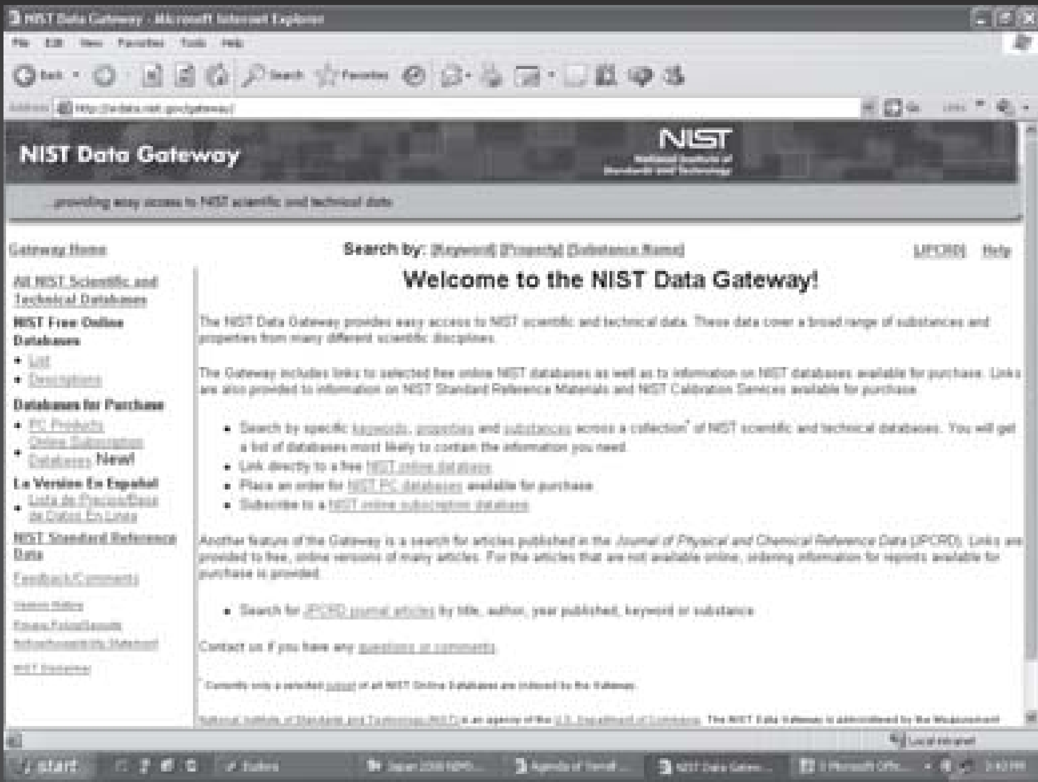
Goal: To make critically evaluated reference data available to scientists, engineers, and the general public

- Analytical Chemistry
- Atomic and Molecular Physics
- Biotechnology
- Chemical and Crystal Structure
- Chemical Kinetics
- Environmental data
- Fire
- Fluids
- International Trade
- Law Enforcement
- Materials Properties
- Optical Character Recognition
- Surface Data
- Text and Video Retrieval
- Thermopysical & Thermochemical

SRD – Customer Access

- NIST Data Gateway-http://srdata.nist.gov/gateway/
- Portal that provides unified access to NIST scientific and technical data
- Customers can search by keywords, properties and substances across a collection of over 100 NIST scientific and technical databases
- Search scope includes articles in the *Journal of Physical and Chemical Reference Data*, plus SRMs and calibration services

Thank you for your attention!



http://srdata.nist.gov/gateway/

Database to Use Materials in High Quality

K. Yagi

National Institute for Materials Science (NIMS),
1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan
YAGI.Koichi@nims.go.jp

1. Introduction

The failure accident of structural components in aged industrial plants increases. The reason is mostly the deterioration of materials due to fatigue, corrosion and so on. The materials are degraded during long service under severe environmental condition. Therefore, it is desired to develop an accurate life prediction method on the base of experimental data, logical knowledge and various experiences.

2. Data and knowledge related to deterioration of materials

The microstructure of material in high temperature service changes, and the deformation behavior is affected by the change in microstructures. And then the nucleation and growth of cavities and cracks are affected by the change in microstructures and the deformation behavior. The change in material properties under creep condition is complicated [1]. Therefore, the information on such time-dependent characteristics as the change in microstructures, the change in damage modes and so on must be prepared in order to predict more accurate remaining life of the structural components used in aged plants.

3. Enriching the contents of database

The creep properties of heat resistant steels are affected strongly by a difference of a very small amount of chemical composition, working ratio and heat treatment condition. Therefore, the creep strength of the steel has a scattering. In the case of the design of high temperature plant, the safety is secured by considering this scattering of creep strength. However, because the steel used are already known in the case of remaining life prediction of used plants, more detailed and more appropriate safety margin should be reconsidered. To estimate the remaining life of the steels used, the data and knowledge concerning the effect of chemical composition on creep strength, the change in microstructures and the nucleation and growth of cavities and cracks must be prepared.

4. Development of database for supporting decision

Because the creep properties of engineering steels are affected largely by a very small amount of chemical compositions, working ratio and heat treatment condition, the creep strength after long service has an uncertainty. Therefore, it is difficult to get a complete solution even if you could accumulate many kinds of data and knowledge. That is, the materials used have a possibility to generate any inexperienced damage and failure modes during long-term service. Therefore, it is required to develop how to use the materials without bringing a large accident even if the damage or failure is happened. It is necessary to introduce a risk-thinking. And it is desired to develop a database which supports the decision for the selection and application of materials on the base of an available risk.

Reference

[1] K. Yagi, .International J. on Pressure Vessel and Piping, 85(2008), 22-29.

MITS 2008 International Symposium
on Materials Database
17 July 2008

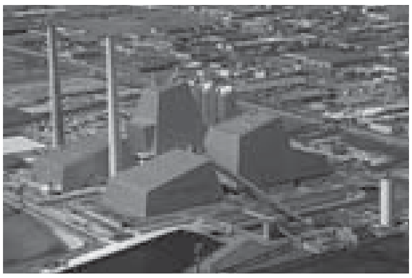
Database to Use Materials in High Quality

K. YAGI
National Institute for Materials Science (NIMS)

I would like to explain using the example of creep strength, which is a kind of material properties at high temperature, that it is important not only to collect experimental data but also to develop and accumulate the knowledge of material properties.

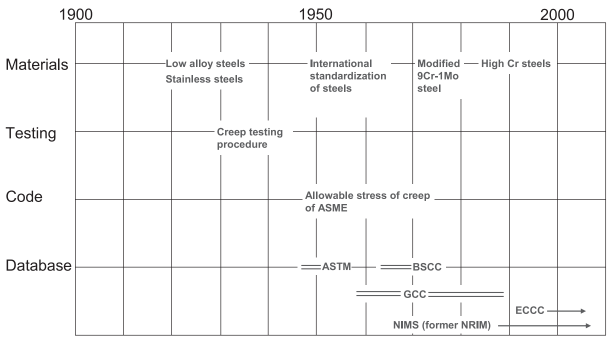
Thermal power plant = Boiler + Turbine + Generator

Because some components in boiler and turbine are exposed in high temperature, **a creep strength** is required for safe use of them.



Avedøre thermal power plant No.1 and No.2 of ENERGI E2 Co. in Denmark

History of acquisition of creep data for heat resistant steels



Allowable stress is provided from the minimum value obtained from the following in ASME Sec. Ⅱ, Part D, Appendix 1;

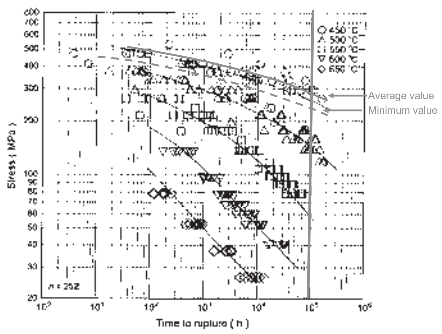
(1) 67% of the average value of 100,000h creep rupture strength

(2) 80% of the minimum value of 100,000h creep rupture strength

(3) 100% of the average value of stress that products a creep rate of 0.01% per 1,000h

⇩

Long-term creep tests must be carried out and long-term creep data of multi-heats of steels and alloys must be acquired from these tests.



Representative Creep Database in the world

☆ **ASTM data series**

Published as part of the Special Technical Publication (STP) in the 1950s

☆ **BSCC high-temperature strength data series**

Complied by British Steelmakers Creep Committee (BSCC) in 1972

☆ **Long-term creep data series by the Iron and Steel Institute of Germany**

on heat resistant steels (carbon steel, low alloy steel, 12Cr steel and stainless steel) was complied in 1968.

Cast steels in 1986

Heat resistant alloys in 1987

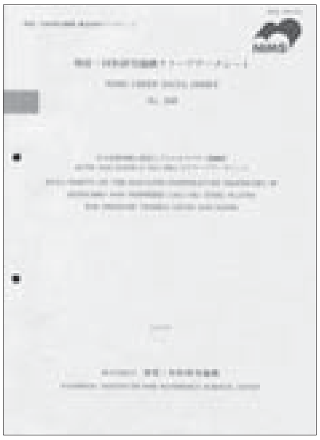
☆ **European Creep Collaborative Committee (ECCC)**

NIMS Creep Data Sheets

National Research Institute for Metals (NRIM), which is the former name of NIMS, started Creep Data Sheet Project at 1966, in order to obtain the 100,000h creep rupture data for heat resistant steels and alloys.

These creep data have been published as a series of NIMS Creep Data Sheets.

Creep testing facilities (Meguro site)



Publication of NIMS Creep Data Sheets

(as of June 2008)

Creep rupture

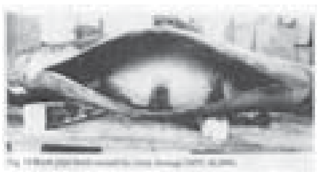
	1st edition	2nd edition	3rd edition	Total
Carbon steels	3	3	2	8
Ferritic steels	24	18	17	59
Austenitic steels	15	13	12	37
Superalloys	11	9	6	26
Total	54	43	34	131

Special edition, No.50 (Match 2004): Long-term creep rupture data (146 data)

Creep deformation

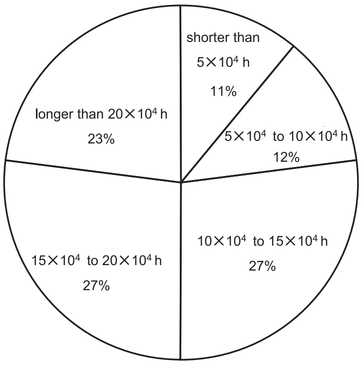
D-1	9Cr-1Mo-V-Nb steels	ASME SA-213/SA-213M Grade T91 ASME SA-387/SA387M Grade 91	March 2007
D-2	9Cr-1Mo-V-Nb steel	ASME SA-387/SA387M Grade 91 Effect of SR heat treatment	March 2008

Cases of creep failure



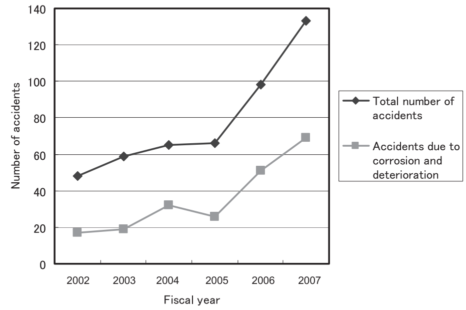
81% of thermal power boiler failure is caused by mechanical damages, and the main cause of mechanical damages is "creep", except abnormal overheat due to operational mistake.

David N. French : "Metallurgical Failures in Fossil Fired Boilers", A Wiley-Interscience Publication, (1983), p.2



Operation time of thermal power plants in Japan

(investigation of November, 1999)



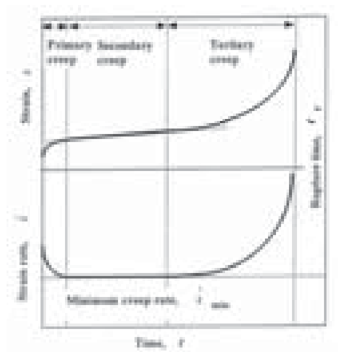
Number of accidents in plants related to High Pressure Gas Safety Law in Japan

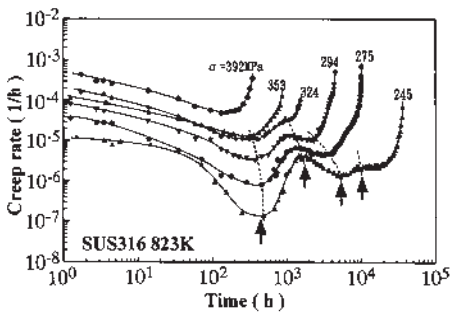
Ageing plants increase

Development of accurate remaining life prediction method for safe and reliable use of ageing plants is needed.

To understand materials deterioration mechanisms based on the change in metallic micro-structures, the material damage etc. is important.

Typical creep curve

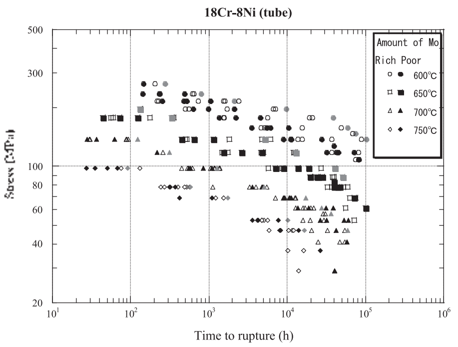


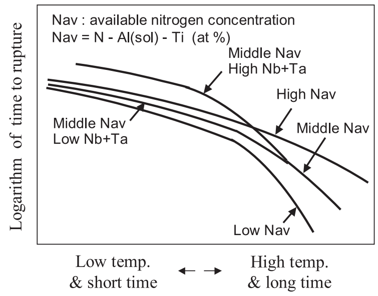


Creep deformation behavior of SUS316 steel

Long-term creep deformation behavior of practical engineering steels and alloys is very complicated.

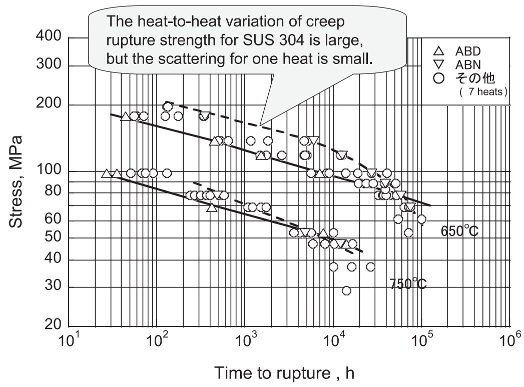
The creep strength is affected by minor chemical elements.





Schematic drawings showing the difference in time to rupture between the heats with high and low Nb+Ta and between the heats with high and low N_{av}.

Creep rupture strength is affected by the difference in a very small amount of minor chemical elements.



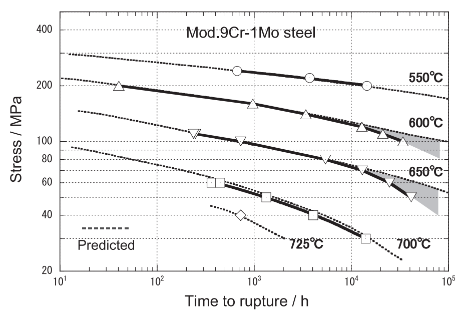
Creep rupture strength of SUS304 steel

A steel has a large scattering of creep rupture strength.

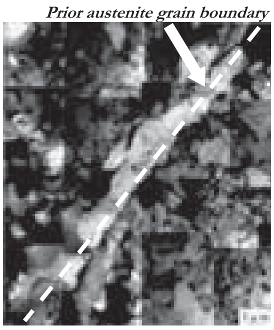
However, the scattering of creep rupture strength in one heat of the steel is small.

↓

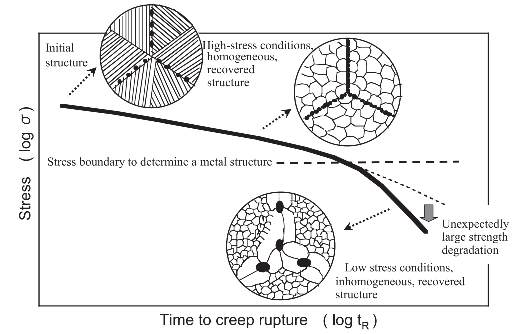
An accuracy of creep life prediction can be improved by understanding the effect of chemical compositions on creep rupture strength and by accumulating the knowledge.



Creep rupture strength of Mod. 9Cr-1Mo steel

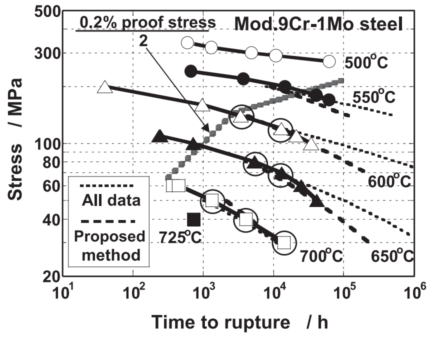


600°C - 100MPa, t_r = 34,141.0h



Schematic illustration on a stress dependence of micro-structural change during creep exposure at the elevated temperatures and its effect on creep strength

Creep life prediction method should be developed based on actual creep strength mechanism of steels.



The creep strength of heat resistant steels is affected by minor chemical elements, heat treatment condition and so on. Furthermore, the strength of structural component is affected by welding.

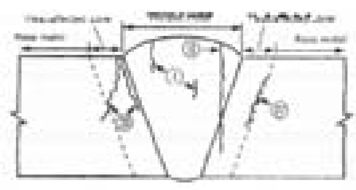
↓

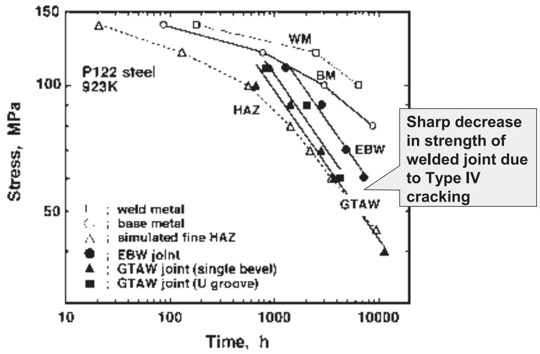
The practical components in a plant has an uncertainty of creep strength.

Creep cracking of welded joint

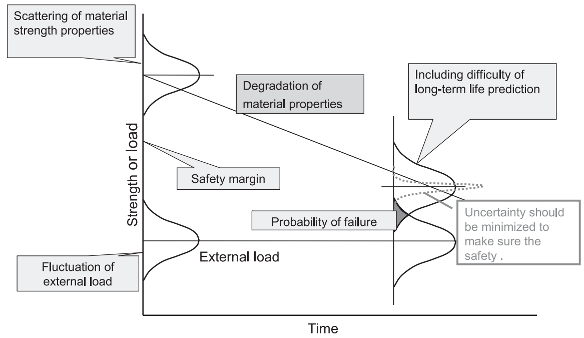
TypeⅣ cracking

Characteristic ; the crack is generated in the inner part under tri-axial stress condition, and the crack propagates from the inner part to outer surface.





Creep rupture times of welded joints of
11Cr-0.4Mo-2W-CuVNb steel



Schematic illustration on probabilistic failure for materials during creep

NIMS Structural Materials Database

- Creep database
- Fatigue database
- Corrosion database
- Space Use Materials Strength database

http://mits.nims.go.jp/

New Database ; information and knowledge to support the application of database

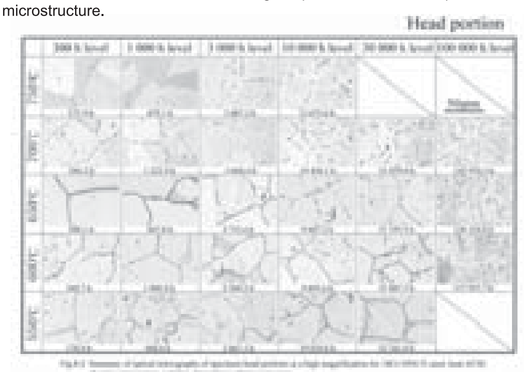
- Micrographs of crept steels
- Materials Risk Information Platform
- Creep data book

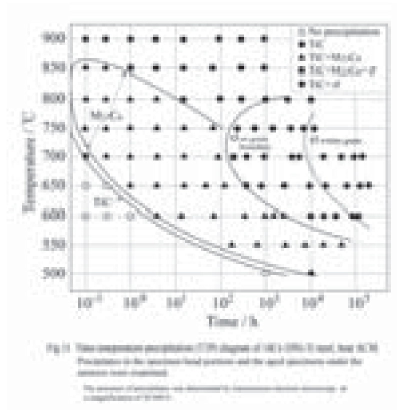
Metallographic Atlas of Long-term Crept Materials

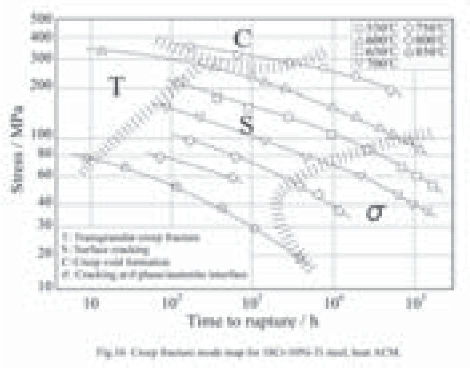
No.	Materials	Designation	Date of publication
M-1	18Cr-8Ni steel	JIS SUS 304HTB	March 31, 1999
M-2	18Cr-12Ni-Mo steel	JIS SUS 316HTB	March 31, 2003
M-3	18Cr-10Ni-Ti steel	JIS SUS 321HTB	March 31, 2004
M-4	2.25Cr-1Mo steels	JIS STBA24 JIS SCMV4NT ASTM A542/A542M	March 31, 2005
M-5	18Cr-12Ni-Nb steel	JIS SUS 347HTB	March 31, 2006
M-6	1Cr-1Mo-0.25V steel	ASTM A470-8	March 31, 2007
M-7	25Cr-20Ni-0.4C steel	SCH22-CF	March 31, 2008

(As of June 2008)

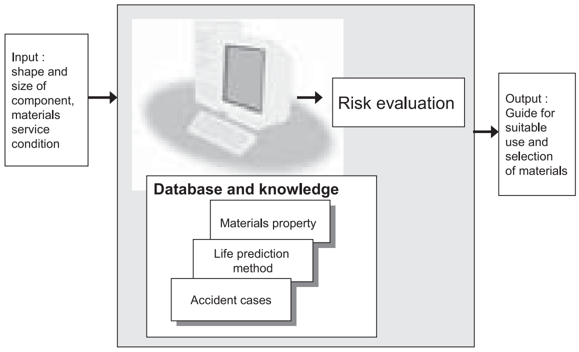
Optical micrographs of specimen head portions at a magnification of 600 for 18Cr-10Ni-Ti steel, heat ACM, showing temperature and time dependence of microstructure.

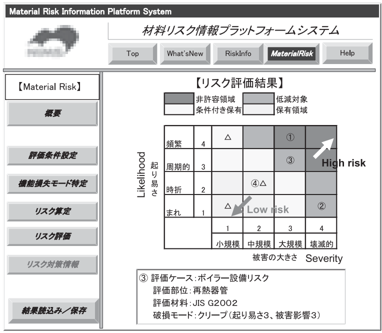






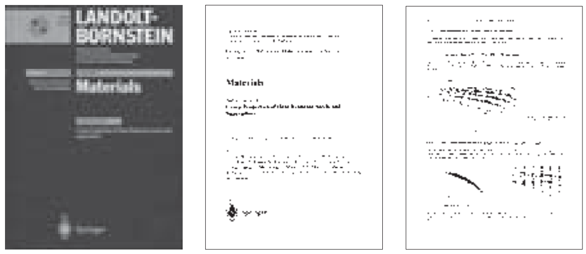
Materials Risk Information Platform

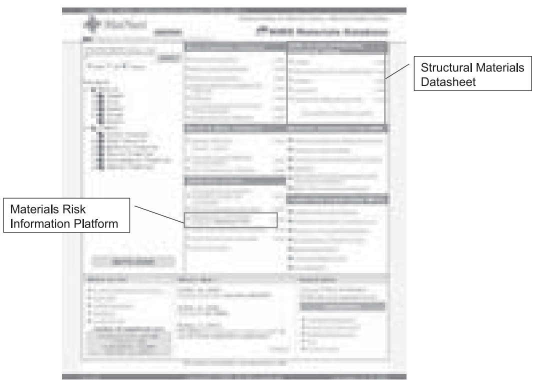




Result of risk evaluation obtained from Material Risk Information Platform System

Publication of "Creep Data Book" under international cooperation of European and Japanese researchers and engineers (2004) ; Creep properties and knowledge for 70 kinds of heat resistant steels and superalloys





Homepage of NIMS Materials Database

http://mits.nims.go.jp

Outline of Structural Materials Database in NIMS Materials Database

Kinds	Publications	
Creep Data Sheet	Data Sheet : No.0	: 1
	No.1～	: 55 (including 1st, A and B editions)
	Technical Document	: 1
	Metallographic Atlas	: 4
Fatigue Data Sheet	Data Sheet : No.0	: 1
	No.1～	: 103
	Technical Document	: 16
Corrosion Data Sheet	Data Sheet : No.0	: 1
	No.1A～	: 4
	Technical Document	: 1
Space Use Materials Strength Data Sheet	Data Sheet : No.0	: 1
	No.1～	: 11

(As of June 2008)

My opinions ;

- To collect reliable data is fundamental for a database.
- Together with aiming to make the unique database, to link the database with worldwide databases effectively is important for the users in the world.
- The material properties is very complicated. Some kinds of knowledge on materials are needed in order to use the data in the database effectively, to understand the material behavior, to select a useful material and to apply the material suitably.
- The information on all sorts of knowledge of materials should be prepared together with making the database.

Thank you very much for your attention.

Materials Database Project in KOREA

B. K. Kim *, Y. M. Rhyim

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66 Sangnam-dong, Changwon, Gyeongnam, 641-010, Korea
* Corresponding author's e-mail address: kbk1649@kims.re.kr

Several years ago, Korean government, the Ministry of Commerce, Industry & Energy (Ministry of Knowledge Economy at present) had framed the policy for promotion of compartment & materials industry in Korea. With regards to the policy, Materials Bank Project has been launched at 2007 for the 5 years program as the first stage. The vision of the materials bank is the world's leading materials data bank as a national infrastructure and its key roles are composed of 3 activities as follows. The first is the construction of combined materials information system for the dissemination of user-oriented information. The second is the international collaboration and network to acquire advanced information on materials and the last is education of materials specialists to secure the R&D competence. The materials bank consists of 3 hubs for metals, chemicals and ceramics respectively, and supervised by the Korea Materials and Components Industry Agency (KMAC; subsidiary organization of ministry of knowledge economy to supervise the national projects such as budget affairs and estimation of research results). The Korea Institute of Materials Science (KIMS) manages the Metals Bank (www.metalsbank.com) as a hub and several national institutes participate as spokes. The Korea Research Institute of Chemical Technology (KRICT) constructs the Chemical Materials Information Bank and Korea Institute of Ceramic Engineering and Technology (KICET) builds the Ceramics Bank. We expect that the materials bank acts as a basis of international collaboration of materials data as well as the promotion of Korean materials industry.

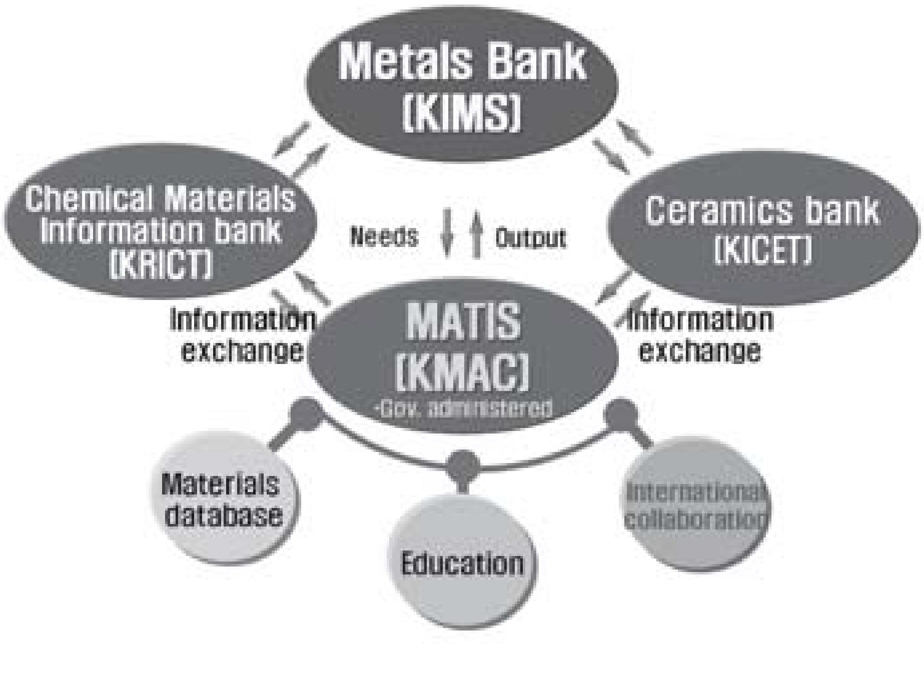
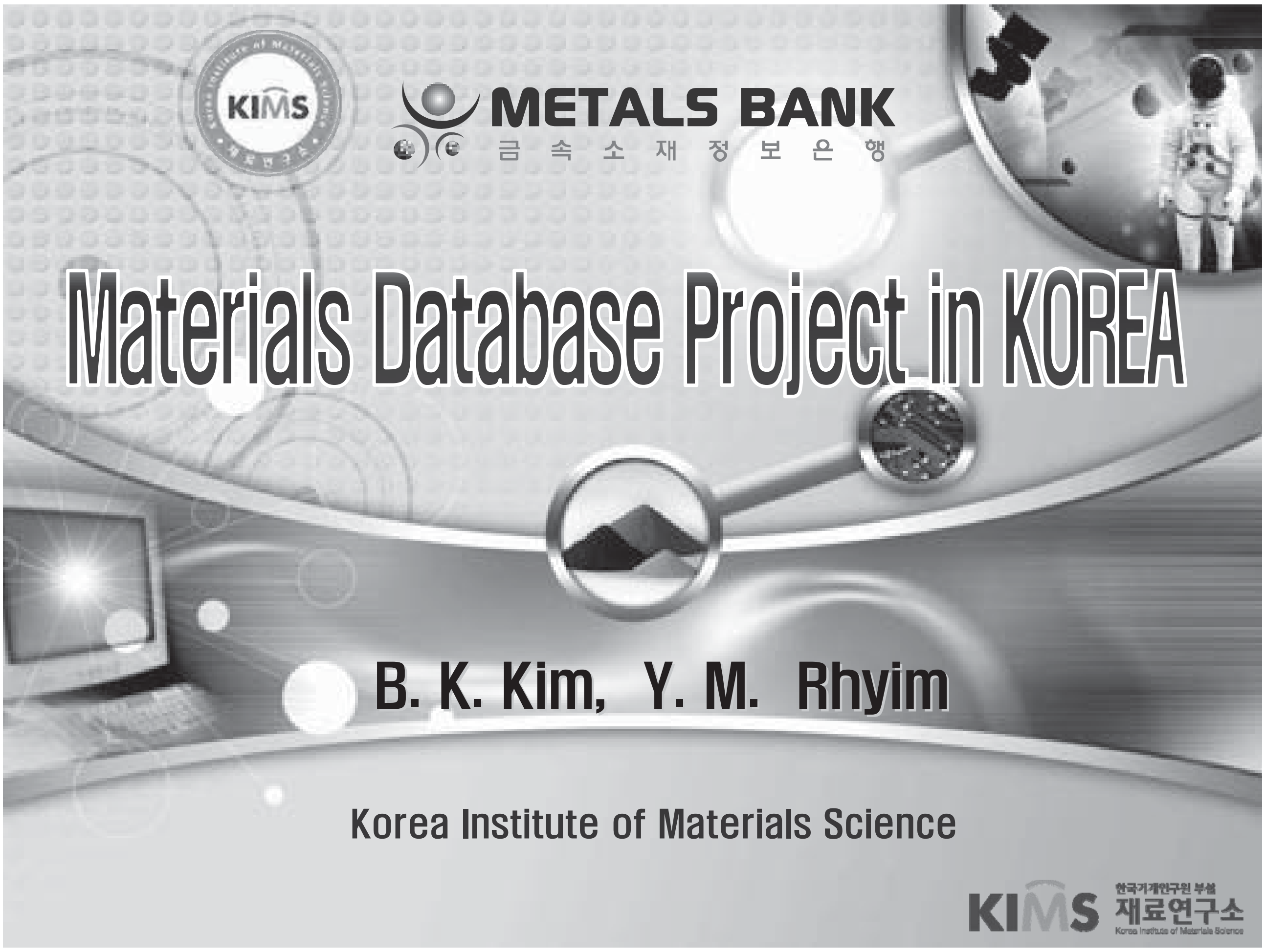


Fig.1 : Constitution and role of materials bank.


KIMS
METALS BANK
금 속 소 재 정 보 은 행
Materials Database Project in KOREA
B. K. Kim, Y. M. Rhyim
Korea Institute of Materials Science
KIMS 재료연구소


Contents
Materials Bank Program – National Project
Introduction of Metals Bank
Introduction of Chemical Material Information Bank
Introduction of Ceramics Bank

Materials Bank Program – National Project

KIMS 한국기계연구원 부설 재료연구소

Background

Necessity

- Needs of Consistent Materials Database for Domestic Materials
- Hub of Materials Related Information as a Representative Agency in Cooperating Network
- Training of Specialists to Secure the R & D capability on the Root Technology

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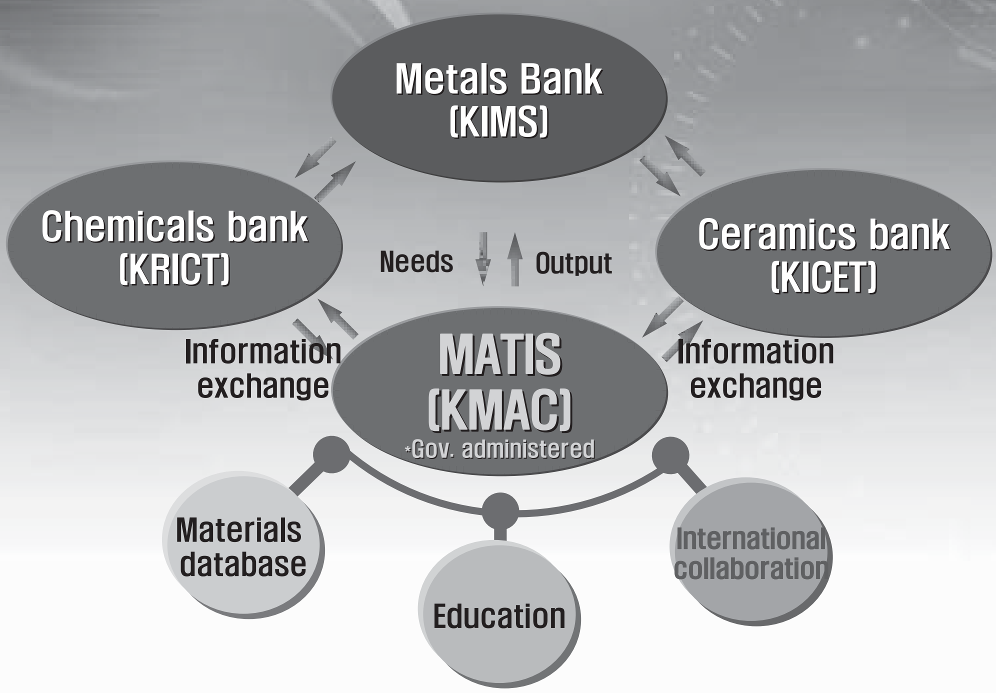
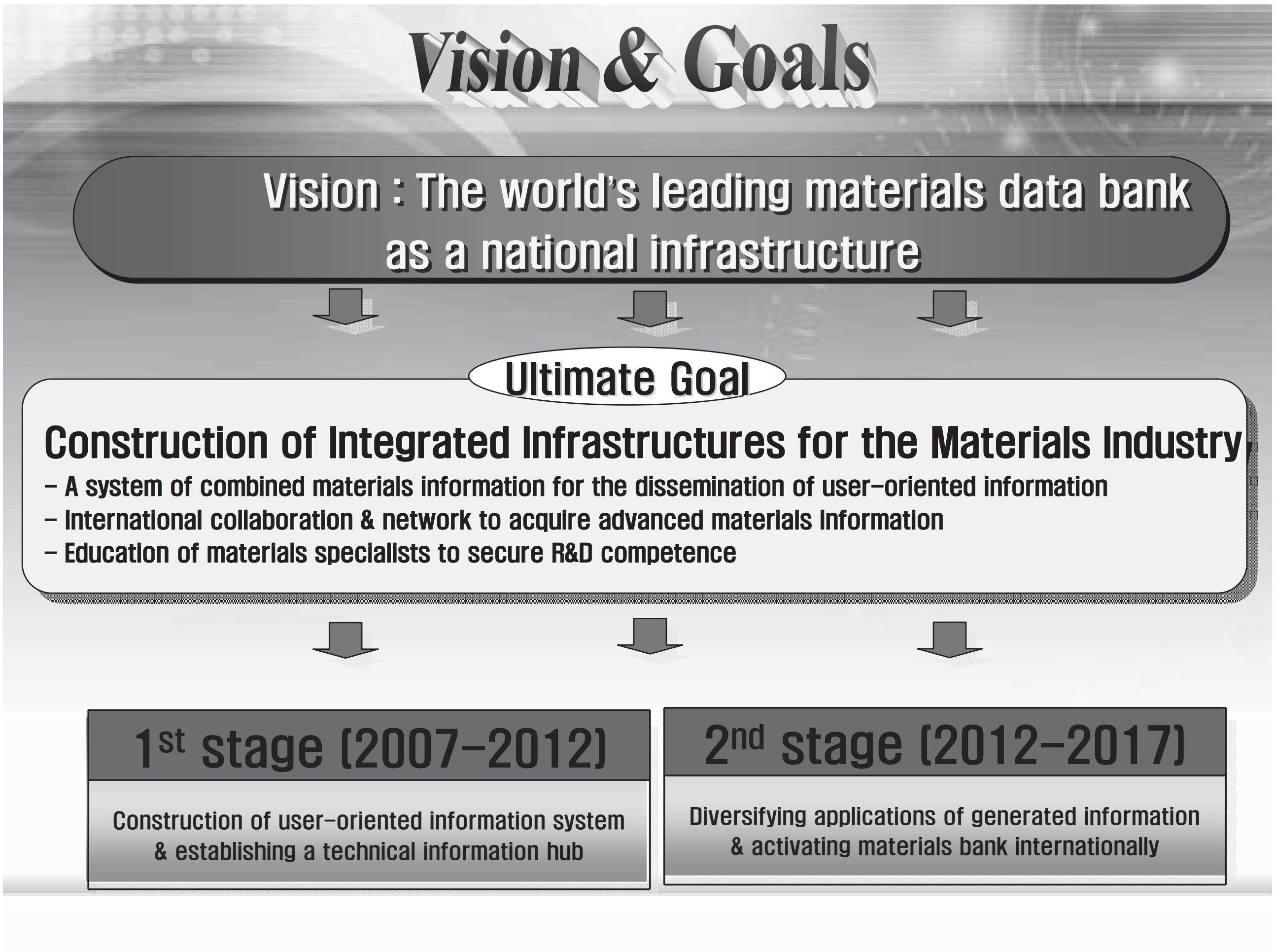
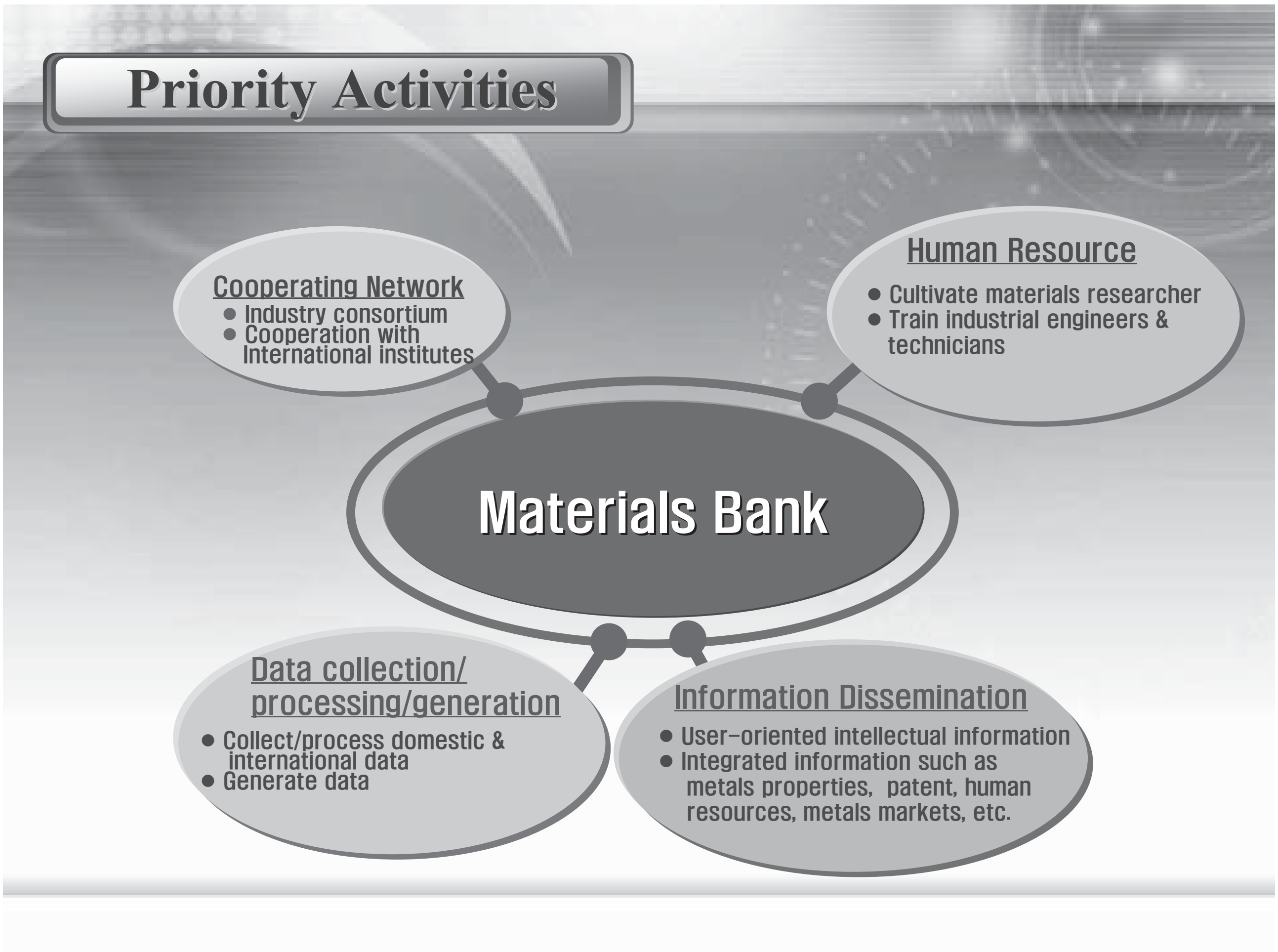
A National Project

- The Materials Bank Project is an Infra Construction
  - A companion program of the materials core technology research program
  - Funding : Ministry of Commerce, Industry & Energy (MOCIE)
    2007 : 7 billion won (~7.4 million USD) will be increased annually
  - Administered by : Korea Materials & Components Industry Agency
  - 1st stage period : 2007.8.1~2012. 7.31
  - Pilot project : Metals bank project (2006.8.1~2007.7.31)

Constitution and role




Vision & Goals
Vision : The world's leading materials data bank as a national infrastructure
Ultimate Goal
Construction of Integrated Infrastructures for the Materials Industry
- A system of combined materials information for the dissemination of user-oriented information
- International collaboration & network to acquire advanced materials information
- Education of materials specialists to secure R&D competence
1st stage (2007-2012)
Construction of user-oriented information system & establishing a technical information hub
2nd stage (2012-2017)
Diversifying applications of generated information & activating materials bank internationally


Priority Activities
Cooperating Network
● Industry consortium
● Cooperation with International institutes
Human Resource
● Cultivate materials researcher
● Train industrial engineers & technicians
Materials Bank
Data collection/ processing/generation
● Collect/process domestic & international data
● Generate data
Information Dissemination
● User-oriented intellectual information
● Integrated information such as metals properties, patent, human resources, metals markets, etc.

Introduction of Metals Bank

HUB : Korea Institute of Materials Science
Director : Vice President Dr. Byung-Kee KIM
Practical staff : Young-Mok RHYIM

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Metals Database

The Priority Order of Metal Species

- The priority of database construction depending on the need of the domestic industry
  - Market needs and core materials of domestic enterprise
  - Industrial demands on the characteristics of materials

- Survey
  - Manufacturers
  - Questionnaire
  - 1:1 interview
- Sphere of selection
  - Car application
  - Used in domestic industry
  - Made in Korea

- DB Structuring
  - Division of Bulk/Powder
  - Unification of characteristic code
  - Basic properties
  - Application properties
  - Durability

- Gathering/ processing
  - ASM Handbook
  - Other DB
  - Paper, report
- Production
  - Self (Metals bank)
  - Collaboration

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Survey : User's Need

Group	Type	Properties
Steel (60 species)	Hot rolled/ Cold rolled	Tensile property, Fatigue property, High strain tensile property, High temperature tensile property, FLD
	STS plate	High temperature tensile property, High temperature low cycle fatigue, Creep-fatigue, Thermo mechanical fatigue, Thermal expansion, Thermal conductivity, Specific heat
Al (10)	Casting alloy Wrought alloy	Tensile property, hardness, Impact energy, Fatigue, Solidus temperature, iquidus temperature, Thermal conductivity, Latent heat
Mg (13)	Casting alloy Wrought alloy	Tensile property, Fatigue property, Creep, Castability, Damping property, High strain tensile property
Powder (20)	Fe base / Cemented carbide	Hardness, Tensile property, Fatigue property, Impact energy, Processing information, Transverse rupture strength

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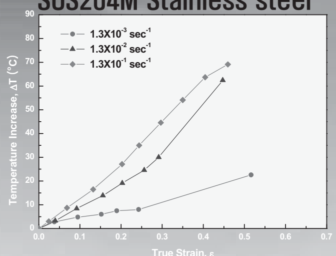
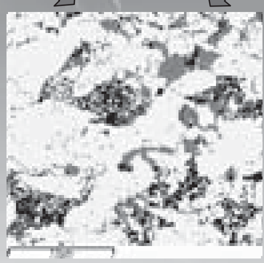
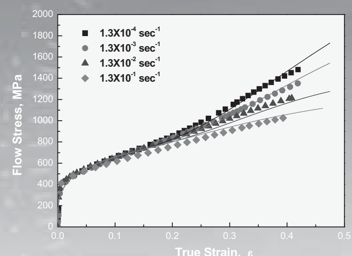
Distinguished feature of DB : Process dependant properties

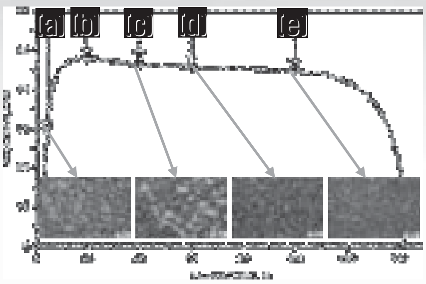
Process history → Phase transformation → Microstructure → Mechanical property

SUS204M Stainless steel









- Material : Mg AZ31B-O Sheet (t=2mm)
- Test temperature : 250°C
- Initial deformation rate : $1x10^{-4}$ sec^{-1}
- Result :
  - (a) : Work hardening due to grain growth
  - (b) – (c) : Work softening by the dynamic recrystallization
  - (d) – (e) : Micro grain boundary sliding

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DB-Structuring : The Structure of KIMS Code

1st Code	Category – Fe : 01, Mg : 02, Al : 03, Powder : 04, …….
2nd Code	Name of the alloy – 6 digit
3rd Code	Manufacturing process– casting, rolling, forging etc. 3 digit
4th Code	Shape – Size and shape – 6 digit
5th Code	Post treatment – heat treatment T4 T5, T6, H24, O, F, etc
6th Code	Properties – Tensile strength, elongation, etc.

Tensile strength of a F heat treated diecating AZ91
; 02-200001-003-001000-001-4101

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Annual Plan for Data Construction

Year	1	2	3	4	5
System H/W	IPS E-learning VOD server	Dual system	Extension	Maintenance	Maintenance
Application S/W	MetCAFE v2.0	MetCAFE v2.1	MetCAFE v2.2	MetCAFE v2.3	MetCAFE v2.4
Data gathering/ processing	Automobile (Steel, Al, Mg) Tool, die material (Cemeted carbide)	Machinery (Steel(rod,wire)) IT (Cu)	Machinery (Steel(rod,wire)) IT (Cu)	Ship (Steel (plate)) Rare earth	Railway (Steel, Al) Rare earth (High T)
Data Production	Durability (fatigue, Creep) : Fe, Al, Mg Application property (cold rolled sheet, Al/Mg casting, cemented carbide, welding)	Application property (cold rolled sheet, Al/Mg casting, cemented carbide, welding)	Durability (Fatigue, Corrosion, Creeo) : Fe, Al, Mg Application property (Hot/cold rolled sheet, Al plate /Mg casting, Cu, cemented carbide, welding)	Application property (SUS/ Hot rolled sheet, Al plate /Mg casting, Cu, cemented carbide, welding)	Application property (Steel rod, casting, Al plate/extruded Mg casting, Cu, cemented carbide, welding)
Propagation	Industry consortium (300, small CAFE)	Industry consortium (400, small CAFE)	Industry consortium (500, small CAFE)		

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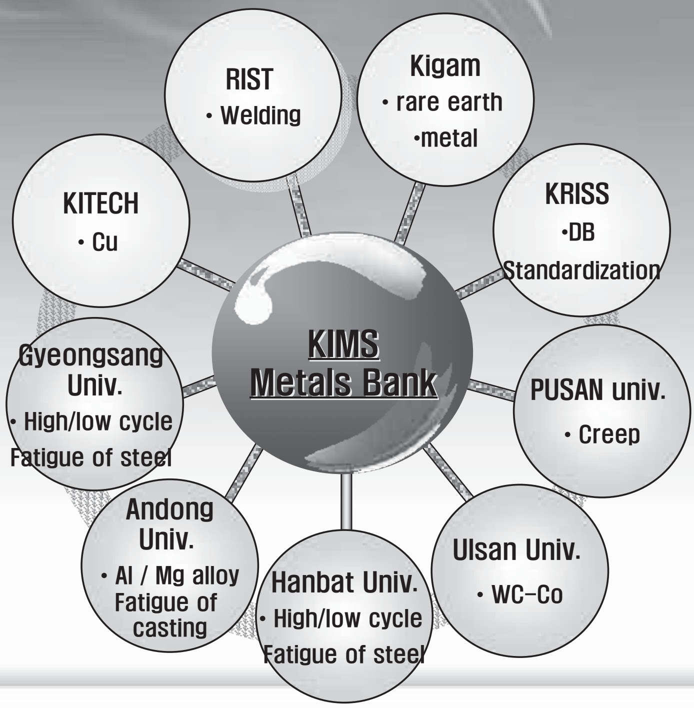
Data Construction Strategy - Cooperation



Organization	Starting year	Data Collection
RIST	1 (2007)	Welding
KITECH	2 (2008)	Electronic/IT (Cu)
KRISS	3 (2009)	Standardization
KIGAM	4 (2010)	Rare earth metal

Univ.	Starting year	Durability
Gyeongsang	1 (2007)	High/low cycle fatigue of steel
Pusan	1 (2007)	Creep
Andong	1 (2007)	Fatigue of Al & Mg alloy
Ulsan	1 (2007)	WC-Co cemented carbide
Hanbat	1 (2007)	High cycle and thermo mechanical fatigue of steel

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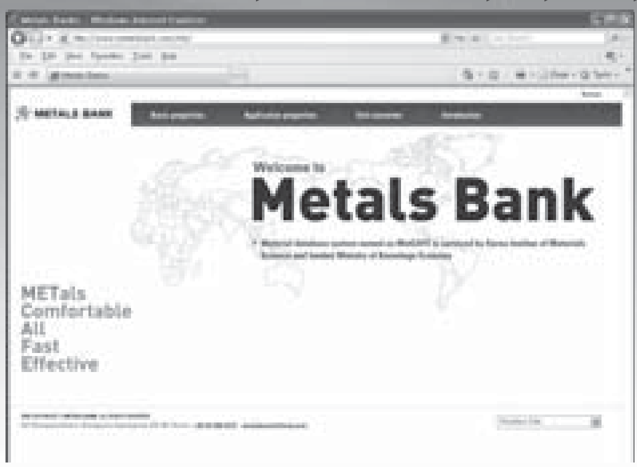
User-Oriented Metals Database

Application S/W : MetCAFE

- www.metalsbank.com
  - Metals, Comfortable, All, Fast, Effective



Homepage (Site map)			
Introduction	Vision & Goal, Priority activity, History		
Metals data	Keyword search		
	Bulk	General search	Basic search
		Advanced search	Composition/property/ complex search
	Powder	Normal Search	Basic/Classified search
		Advanced search	Composition/property/ complex search
	Application property	Compression, Tensile, Fatigue Creep, FLD, Data Book	
	Unit converter		
Other Inform	Patent, Market, Personnel, Technology trend		
Education	e-learning		
User	Newsletter, Notice, FAQ, Q&A, etc.		

- Keyword search, General search, Advanced search, Classified search
  - Materials selection function

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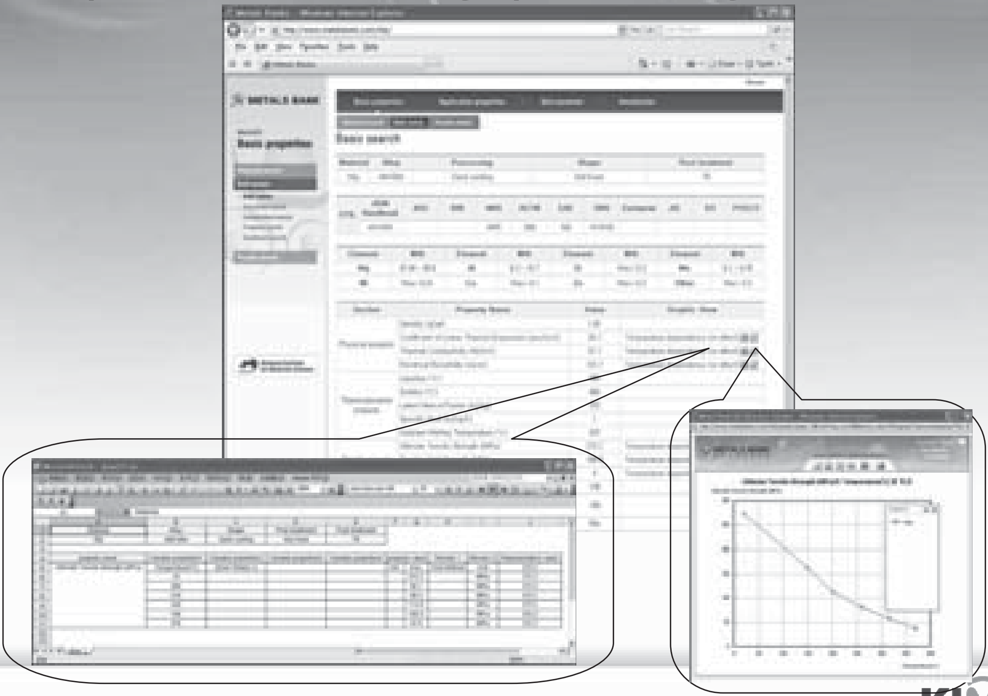
Flexible to User's Demand

- All data digitalized
  - can be presented as text or graph, according to the user's demand



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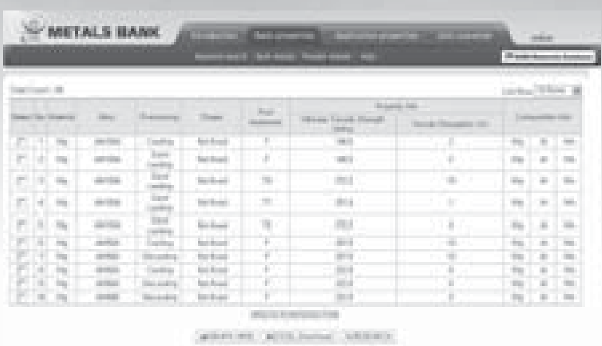
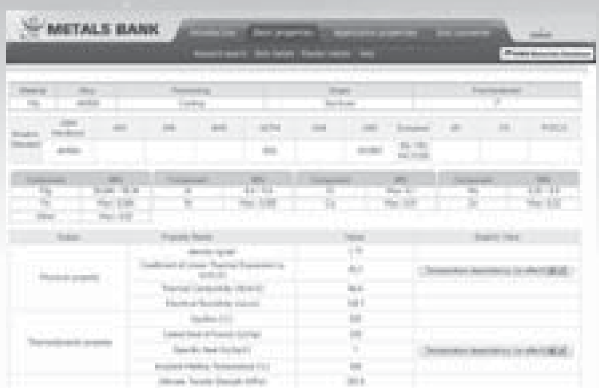
Current Status

Materials Category	Type	Number of data
Steel (177 species)	Hot rolled/Cold rolled/STS plate	20,915
Mg (30)	Casting alloy Wrought alloy	7,390
Al (71)	Casting alloy Wrought alloy	5,646
Powder (20)	Ferrous powder	4,194





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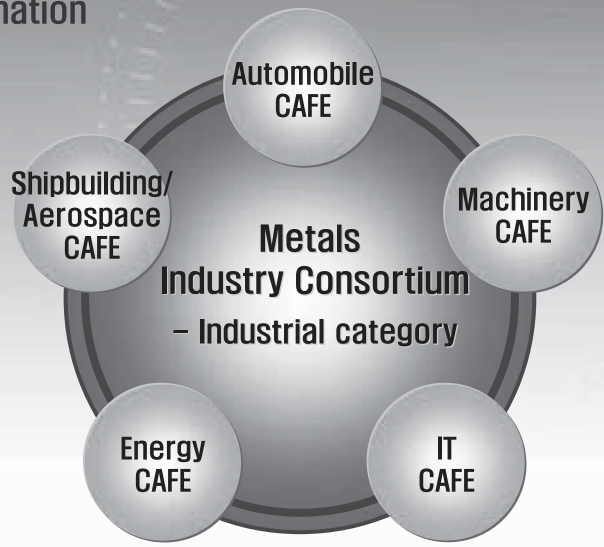
Information Dessemination

- Related Industry Consortium (284 companies)
  - Investigation on DATA requirement
  - Closed service of high level information

* Component company : 208
* Materials company : 54 (POSCO etc.)
* End product company : 13
  (Hyundai-motor, LG electronics, etc.)
* The others : 9
  (Engineering, Testing etc.)



- Classified Small Café Activity
  - Promotion of cooperation between industry, Institute, and University

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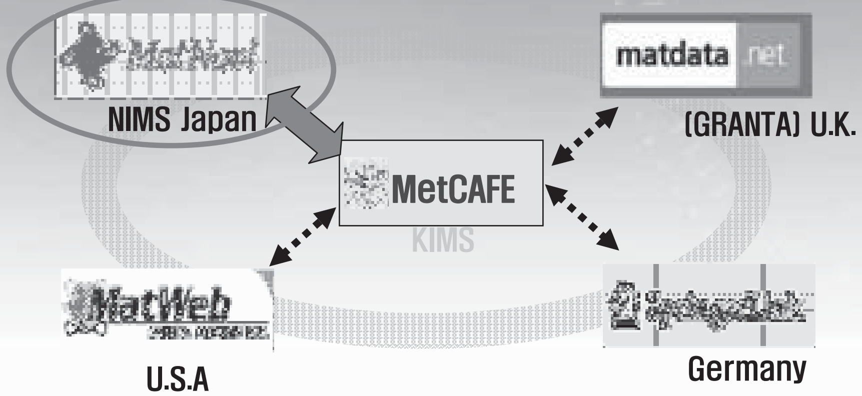
International Collaboration

- Networking with International metals banks for cooperation
  - International institutes : 14 institutes in 8 countries
    NIMS (Japan), NIST (USA) GKSS (Germany), etc.
  - International technical networking establishing an online global Hub
  - Data exchange for core technology development of specific materials and technology adoption



- Korean focal point of metals information
  - Connection/Cooperation with overseas metals database
  - Technology networking with overseas materials research institutes

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Cultivating Metals Experts

- Training next generation researchers for R&D competence
  - Graduate student centered, training on basic theory and research
  - Cooperation with universities
  - International cooperation
- Short course for Industrial workers
  - Technology oriented education programs
- Contracting MOU with 9 Universities on training specialists

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Development of E-learning System

- Cyber education service (on-line)
  - 5 topics available as of January 2008

KIMS 한국기계연구원 부설 재료연구소

Introduction of KIMS

Location

The city of Changwon, southern part of south KOREA

Mission and History

Mission

KIMS(Korea Institute of Materials Science), the Government funded research institute, is established to plan, research & develop, test & evaluation and provide technical support in the field of materials and to promote the advancement of the nation's science and technology.

History

- 1976.12.30 : The Korea Institute of Machinery and Metals (KIMM) was founded in Changwon.
- 1992. 3.16 : The Main office of KIMM was moved from Changwon to Taeduk.
- 1995. 9. 1 : Fullname of KIMM was partly changed ‘Metals’ into 'Materials'
- 2002. 3. 1 : Changwon station was named as Materials Research Institute.
- **2007. 4.27 : The Korea Institute of Materials Science was founded** as a subsidiaries of KIMM.

KIMS 한국기계연구원 부설 재료연구소

Organization

- President
  - Vice President
    - Department of Advanced Metallic Materials
    - Department of Materials Processing
    - Department of Surface Technology
    - Department of Powder Materials
    - Department of Test and Evaluation
    - Future Technology Center
  - Department of Planning and R&D Management
  - Department of Administration Management

- **Total number of regular staffs: 202**
  - **- Researcher : 138 , Engineer : 40, Administrator : 24**
- **Number of research assistants: 169**

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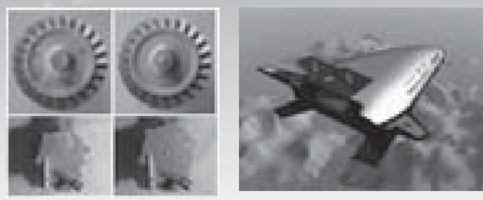
Reserch Field

Advanced Metallic Materials Technology

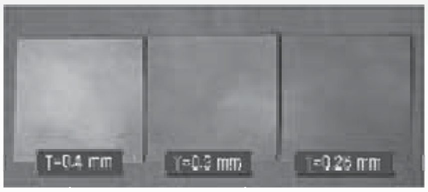
Development of global leading technology in new metallic materials for structural applications.

- High Nitrogen Stainless Steels
- High Temperature Superalloys
- High Performance Light Metals

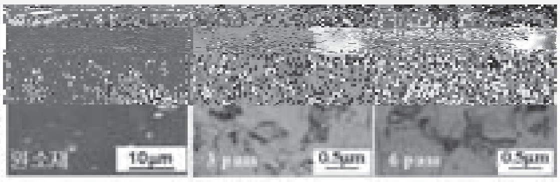
High strength multiphase steel



Next generation high-temp. alloy



Magnesium alloy hot and cold rolled sheets



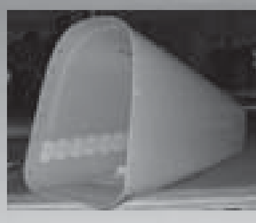
Grain refinement of aluminum alloys

KIMS 재료연구소

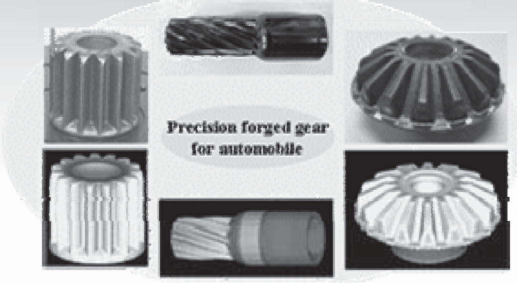
Materials Processing Technology

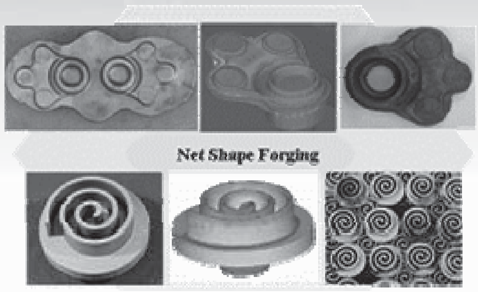
Development of advanced processing and forming technology of metals and fiber reinforced plastic composites for commercialization.

- Precision Forming and Near-Net Shape forming
- Structural Design and Evaluation of Composites
- Microstructure Control of Ni-based and Ti-based Alloys



Resin Transfer Molding





Precision Forged Parts

KIMS 재료연구소

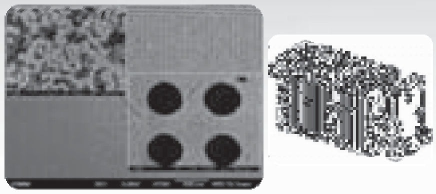
Surface Technology

Development of Core Technology in Surface Modification for Next Generation 5T (IT, BT, NT, ET, ST) Industry.

- **Surface Coating by Dry/Wet Processes**
- **Thin Films for Flexible Displays and Solar Cells**
- **Surface Modification for Biomedical Applications**
- **Stacks and Their elements of Fuel Cells**

Industrial applications of thin film coatings

Transparent conducting oxide thin films



Porous electrode and stack of fuel cell

KIMS 한국기계연구원 부설 재료연구소

Powder Materials Technology

Development of High Performance Powder Materials and Components by Making Multi-Functional Nano-Size Powders and by Using Special Shaping and Sintering Methods.

- **Fabrication of mixed fine powders for structural and functional applications**
- **Advanced ceramic materials for structural and ecological applications**
- **New functional powder materials for energy conversion**

[Automobile parts]

[Tools & dies]

[Bio applications]

[Energy applications]

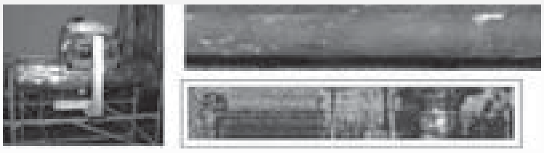
KIMS 한국기계연구원 부설 재료연구소

Test and Evaluation Technology

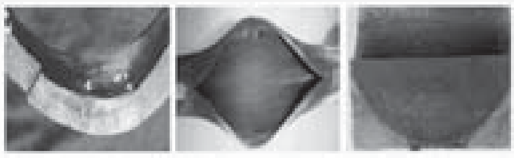
Development of Testing and Evaluation Technology of Various Advanced Materials and Performance of Authorized Inspection of Nuclear Power Plants as well as Failure Analysis of Industrial Parts.

- **High quality evaluation of materials' properties and their nano-scale characterization**
- **Failure analysis and life prediction of parts**
- **Authorized inspection of nuclear plants**
- **Calibration of instruments**

Authorized Inspection of Nuclear Plant



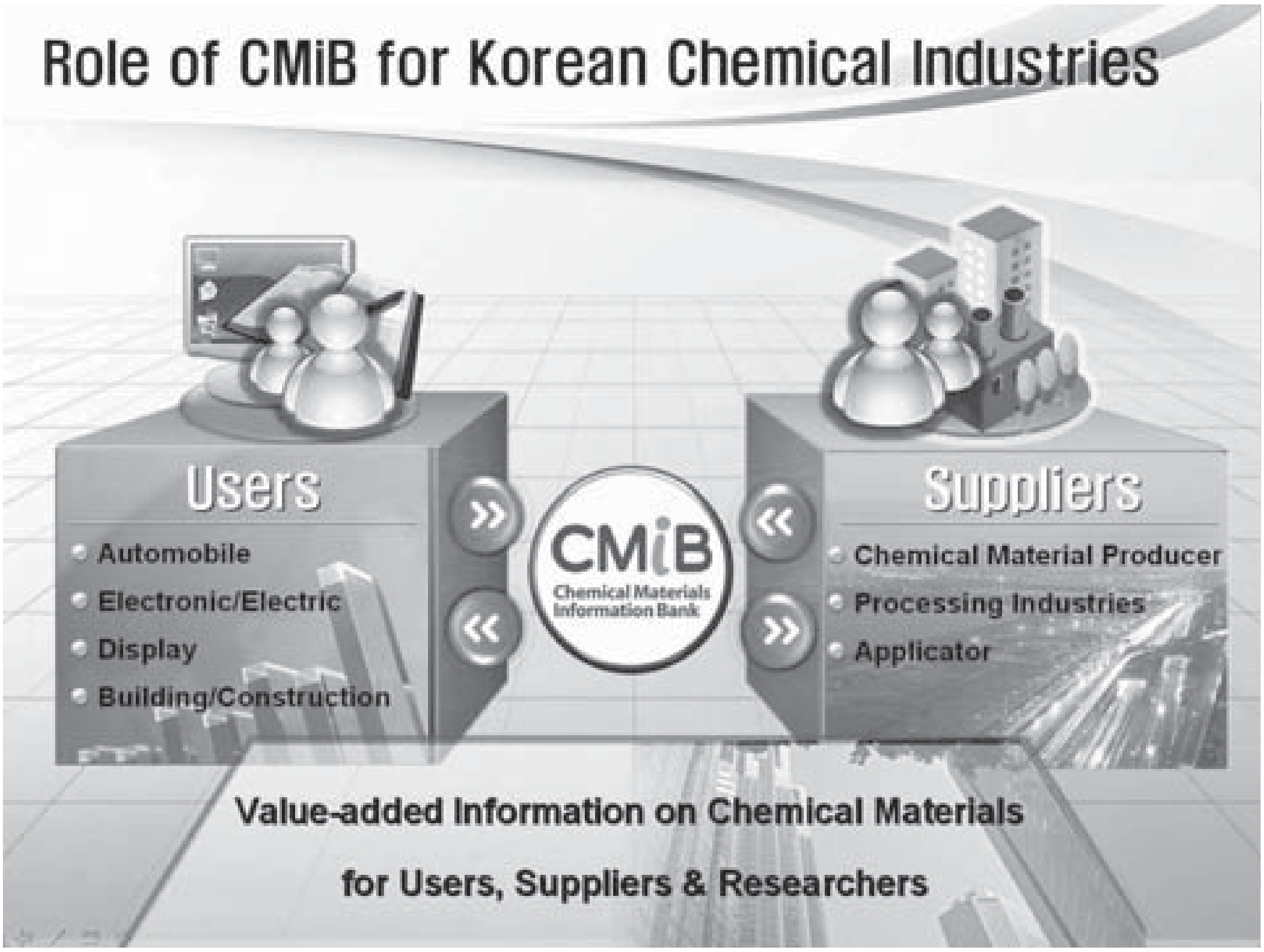
Automatic On-line Thickness Measurement of Pipeline using Radioisotope

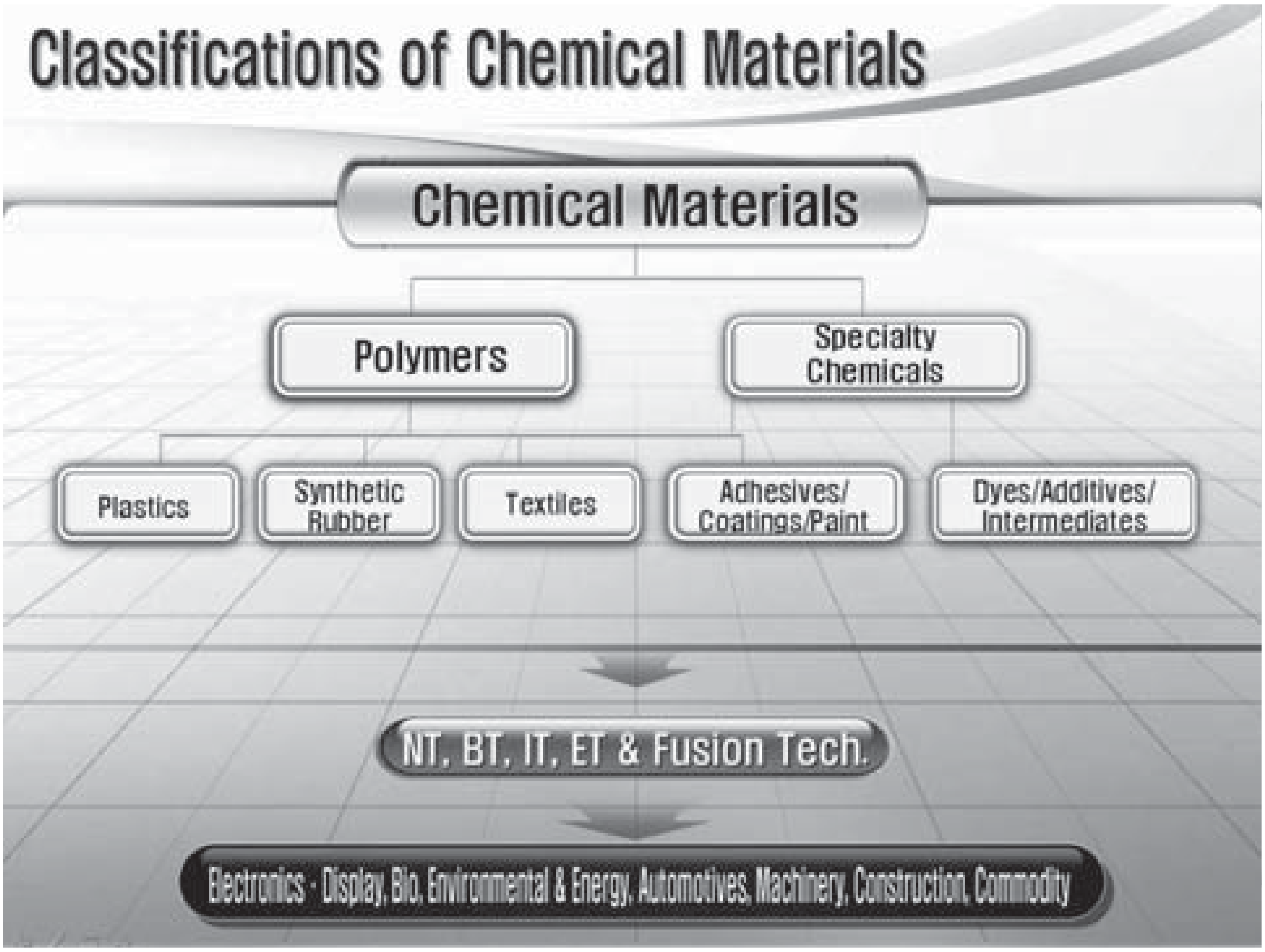


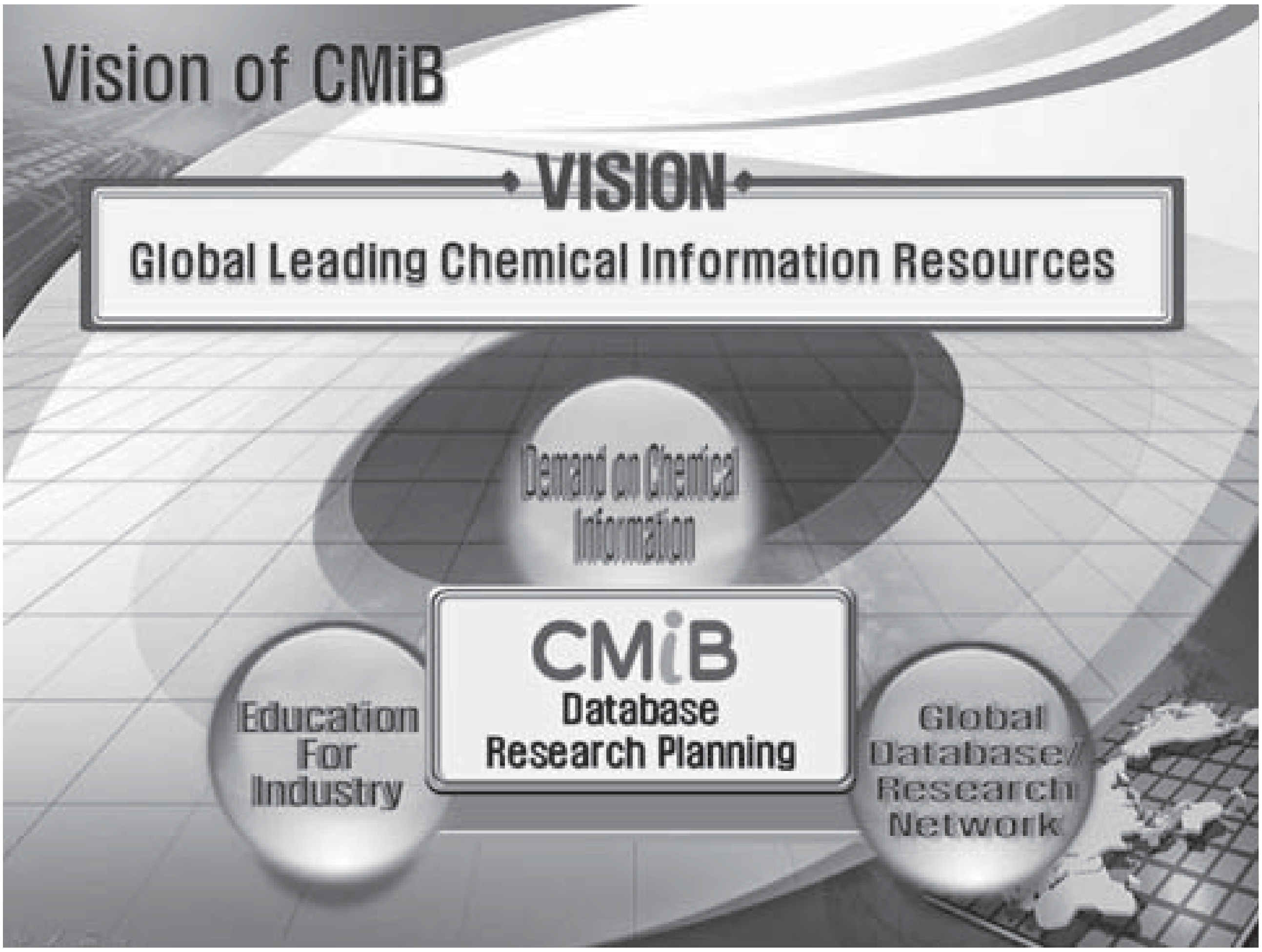
Failure Analysis of a Boiler Tube

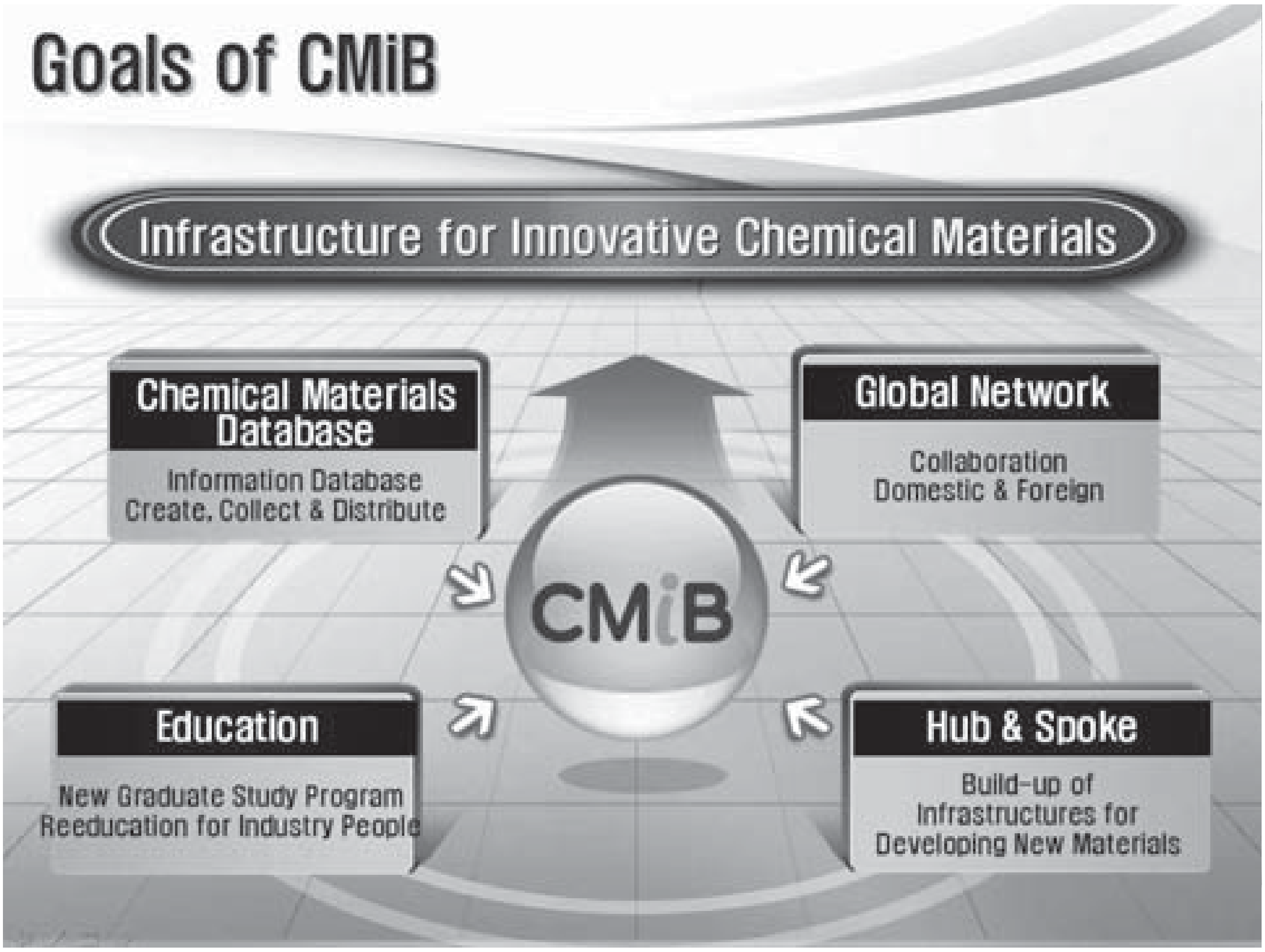
Introduction of CMiB

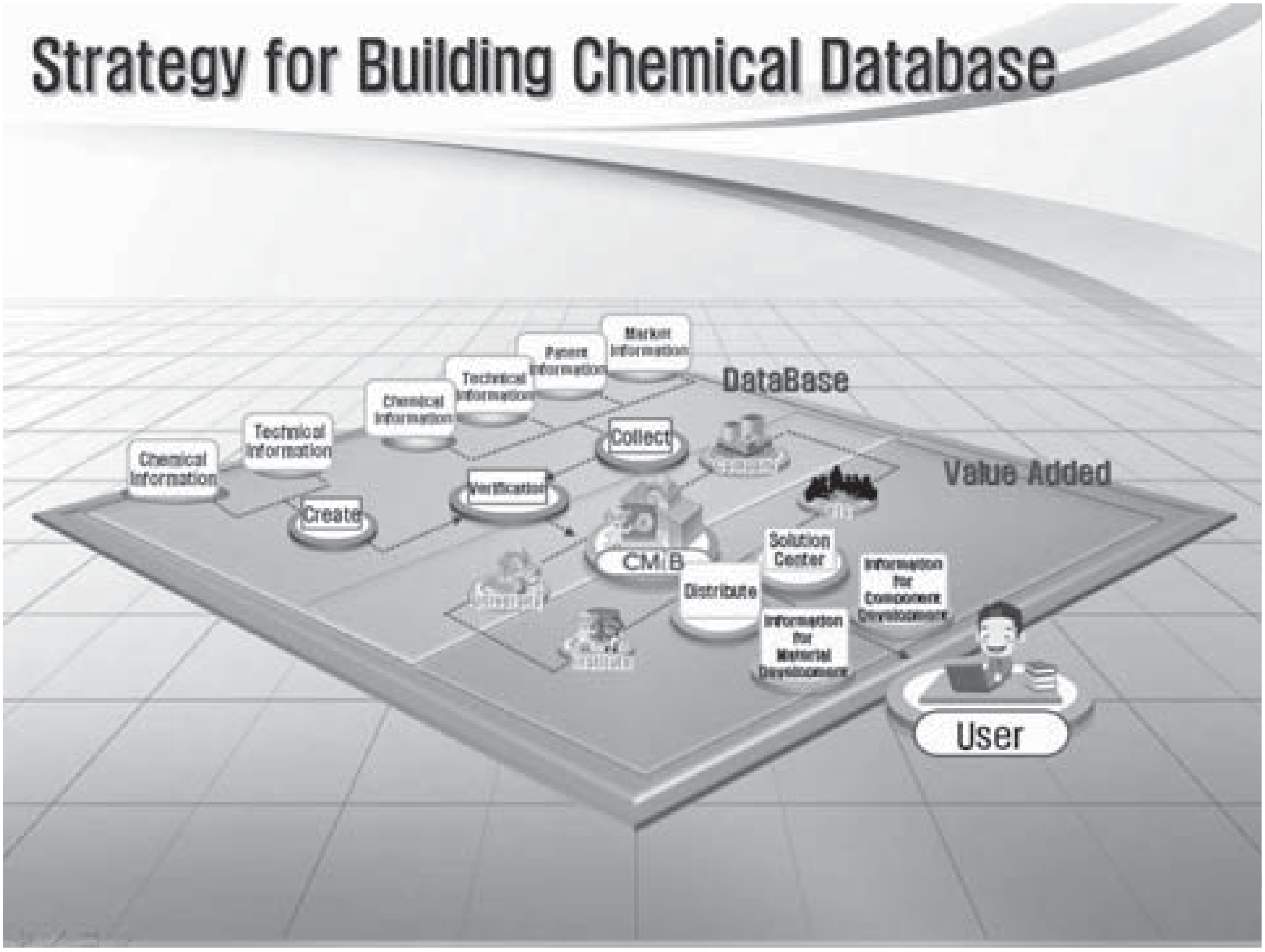
HUB : Korea Research Institute of Chemicals Technology
Director : Vice President Dr. Jae-Heung LEE
Practical staff : Dr. Sung-Goo LEE (sglee@krict.re.kr)

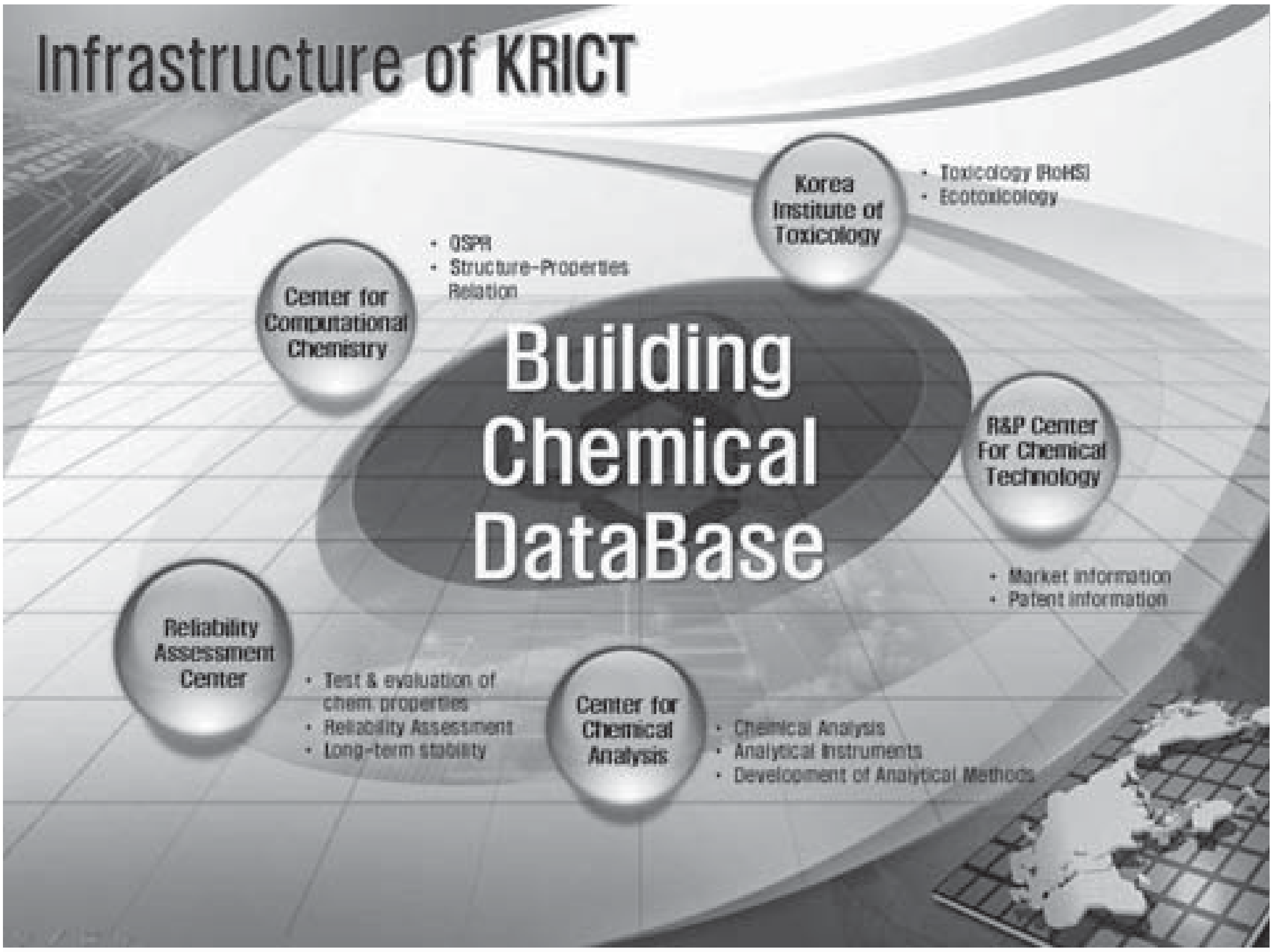

Role of CMiB for Korean Chemical Industries
Users
Automobile
Electronic/Electric
Display
Building/Construction
CMiB
Chemical Materials Information Bank
Suppliers
Chemical Material Producer
Processing Industries
Applicator
Value-added Information on Chemical Materials
for Users, Suppliers & Researchers

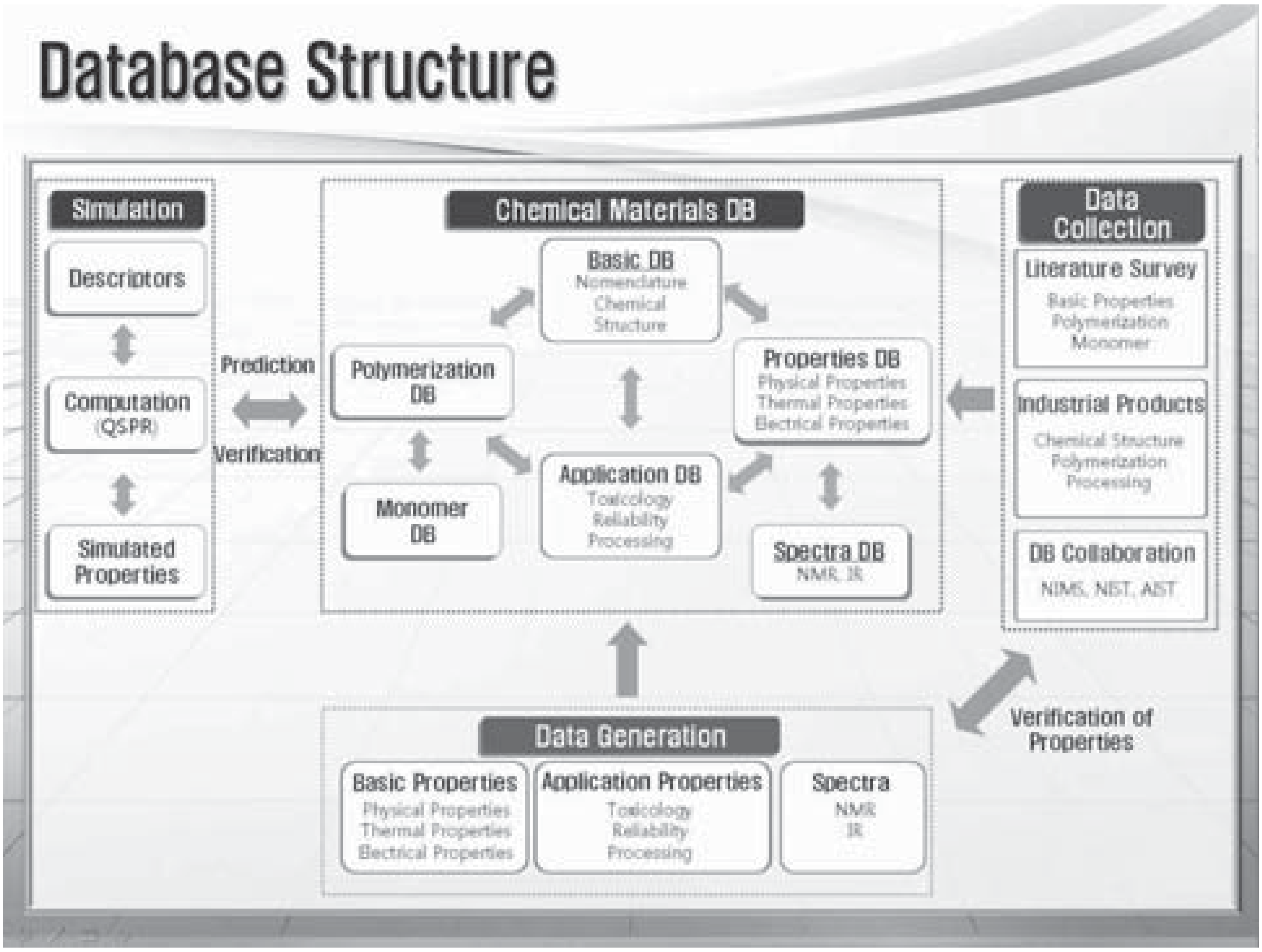

Classifications of Chemical Materials
Chemical Materials
Polymers
Specialty Chemicals
Plastics
Synthetic Rubber
Textiles
Adhesives/ Coatings/Paint
Dyes/Additives/ Intermediates
NT, BT, IT, ET & Fusion Tech.
Electronics · Display, Bio, Environmental & Energy, Automotives, Machinery, Construction, Commodity

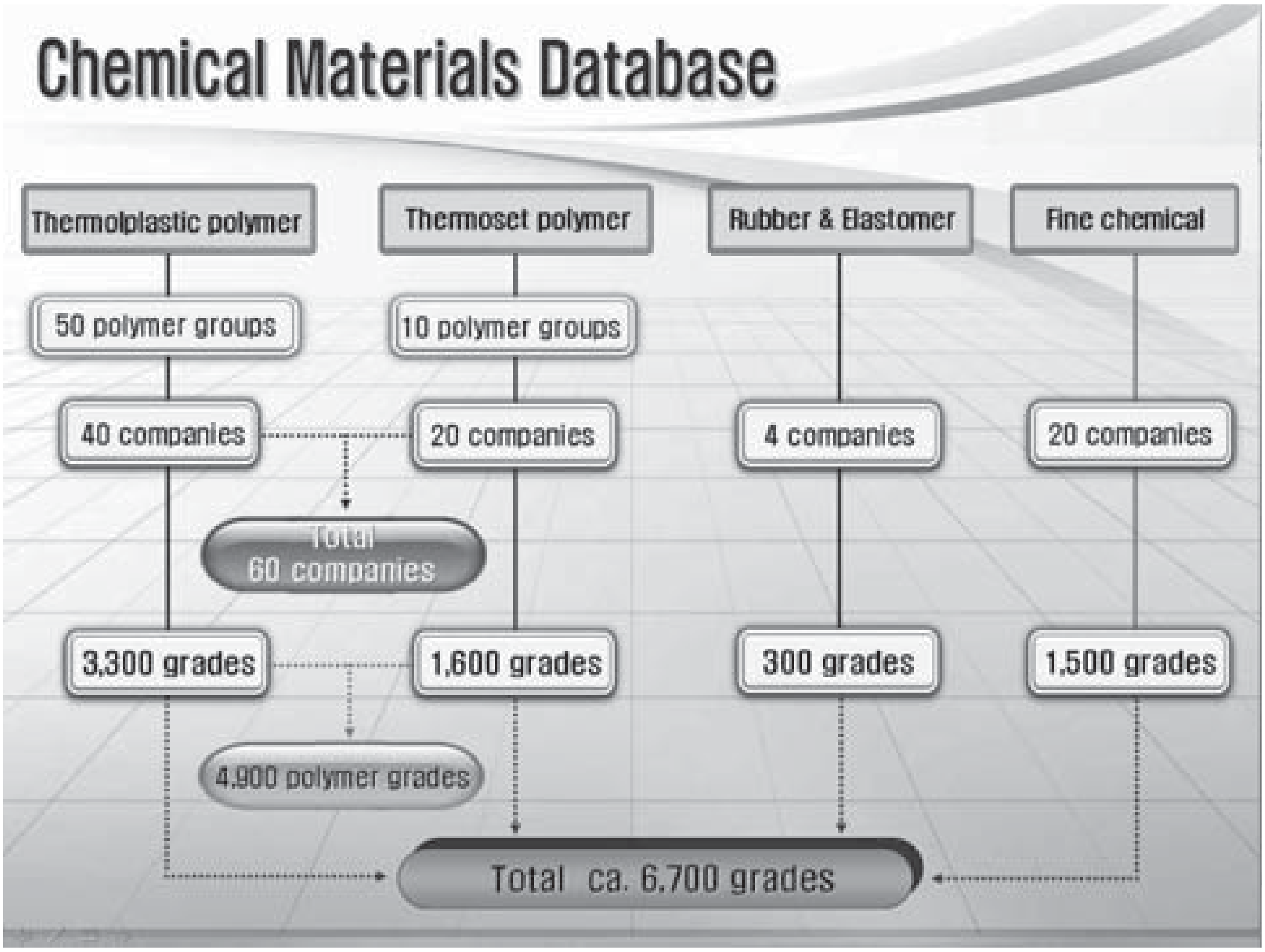

Vision of CMiB
VISION
Global Leading Chemical Information Resources
Demand on Chemical Information
CMiB
Database
Research Planning
Education For Industry
Global Database/ Research Network

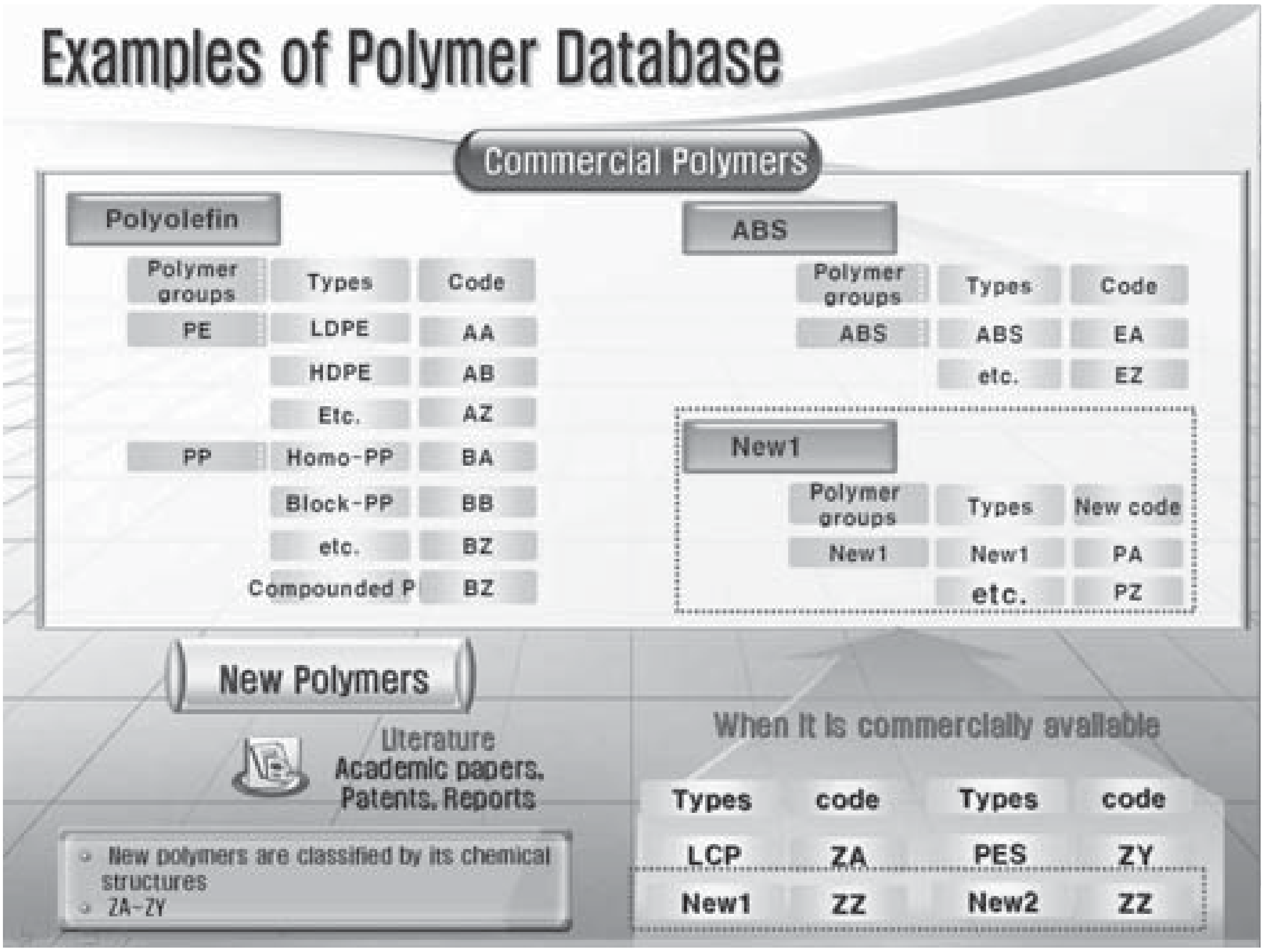

Goals of CMiB
Infrastructure for Innovative Chemical Materials
Chemical Materials Database
Information Database
Create, Collect & Distribute
Global Network
Collaboration
Domestic & Foreign
CMiB
Education
New Graduate Study Program
Reeducation for Industry People
Hub & Spoke
Build-up of
Infrastructures for
Developing New Materials

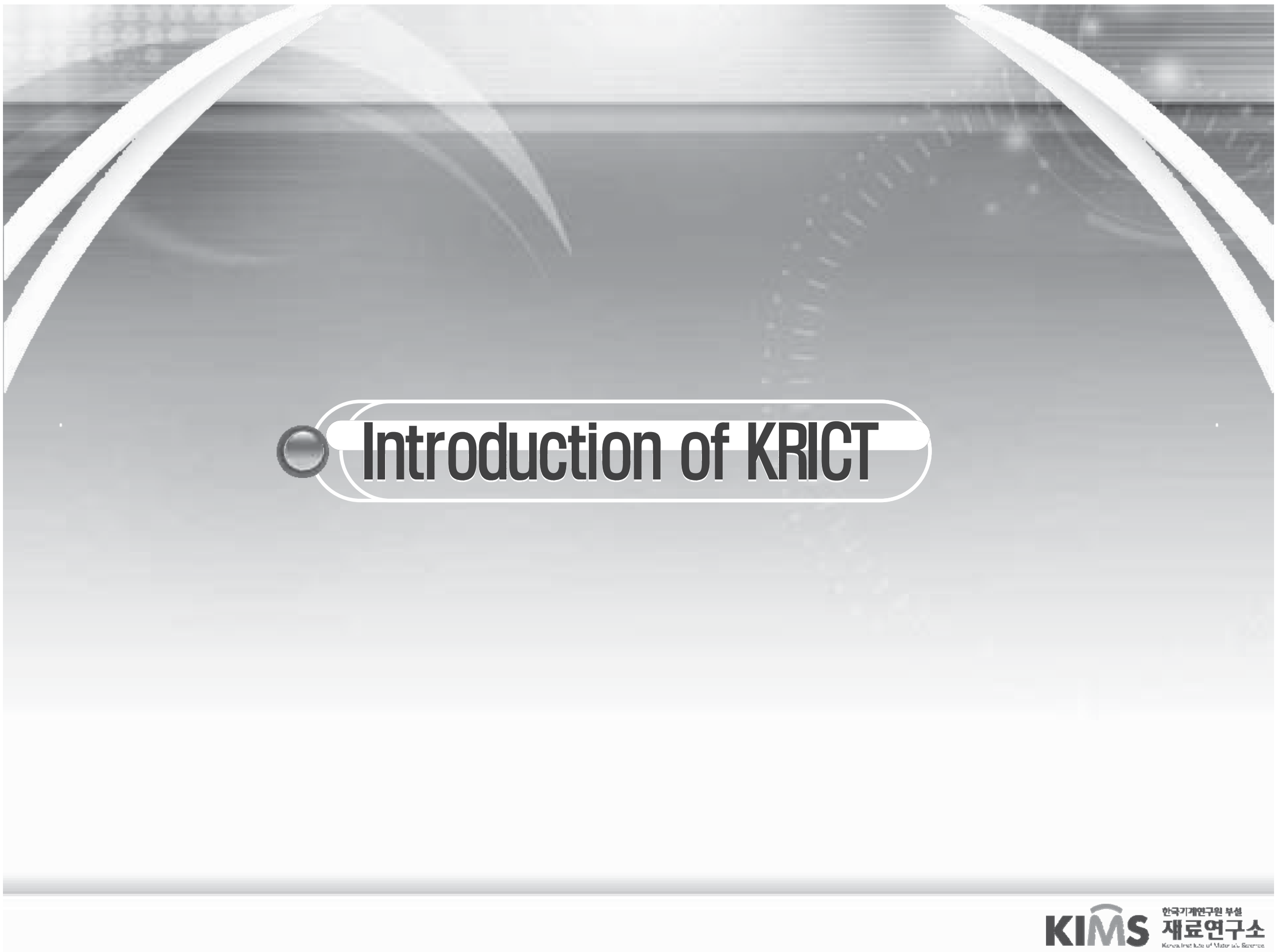

Strategy for Building Chemical Database
Market Information
Patent Information
Technical Information
Chemical Information
DataBase
Technical Information
Chemical Information
Collect
Value Added
Verification
Create
Solution Center
CMIB
Information for Component Development
Distribute
Information for Material Development
User

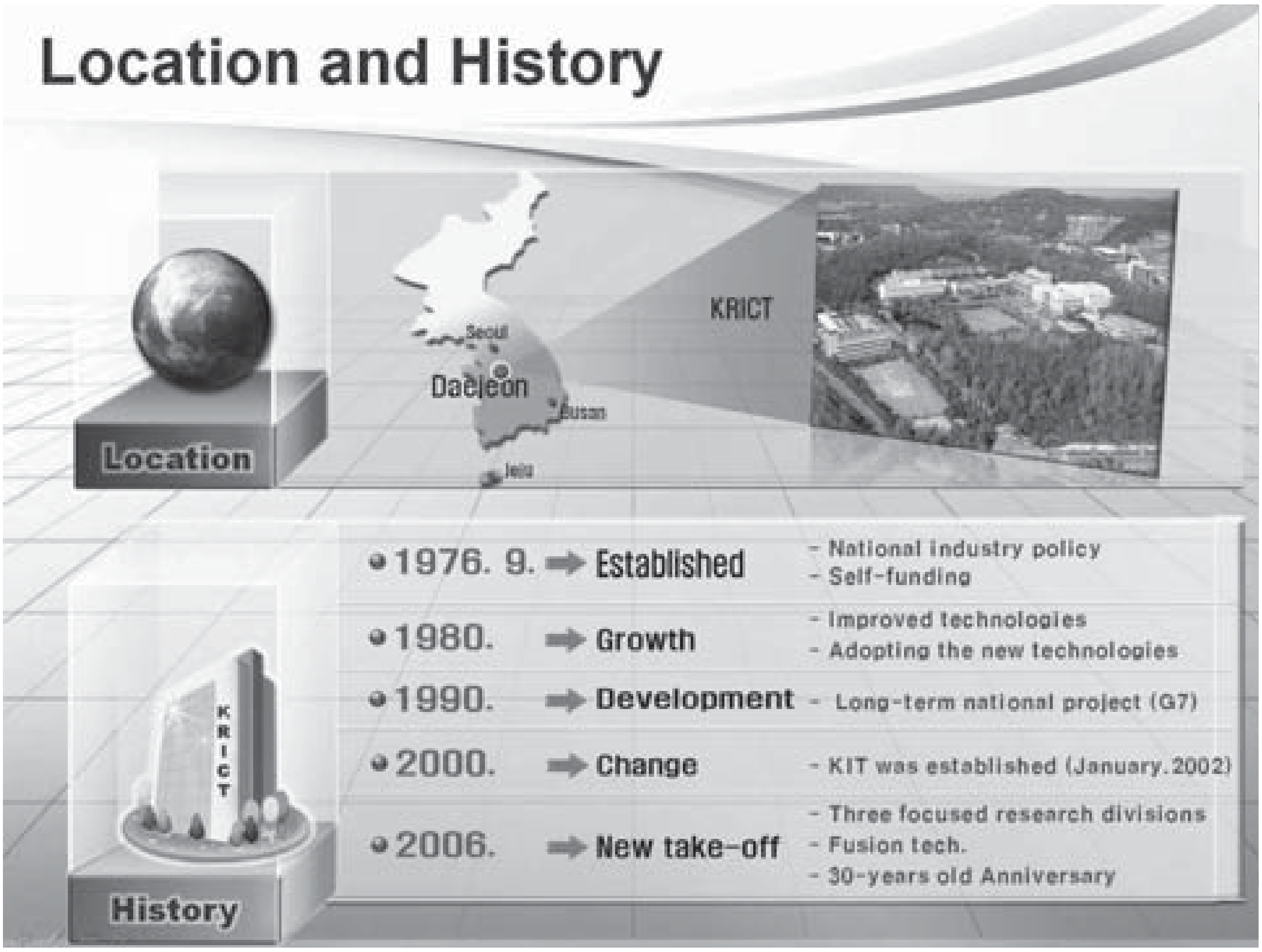

Infrastructure of KRICT
Korea Institute of Toxicology
• Toxicology (RoHS)
• Ecotoxicology
Center for Computational Chemistry
• QSPR
• Structure-Properties Relation
Building Chemical DataBase
R&P Center For Chemical Technology
• Market information
• Patent information
Reliability Assessment Center
• Test & evaluation of chem. properties
• Reliability Assessment
• Long-term stability
Center for Chemical Analysis
• Chemical Analysis
• Analytical Instruments
• Development of Analytical Methods

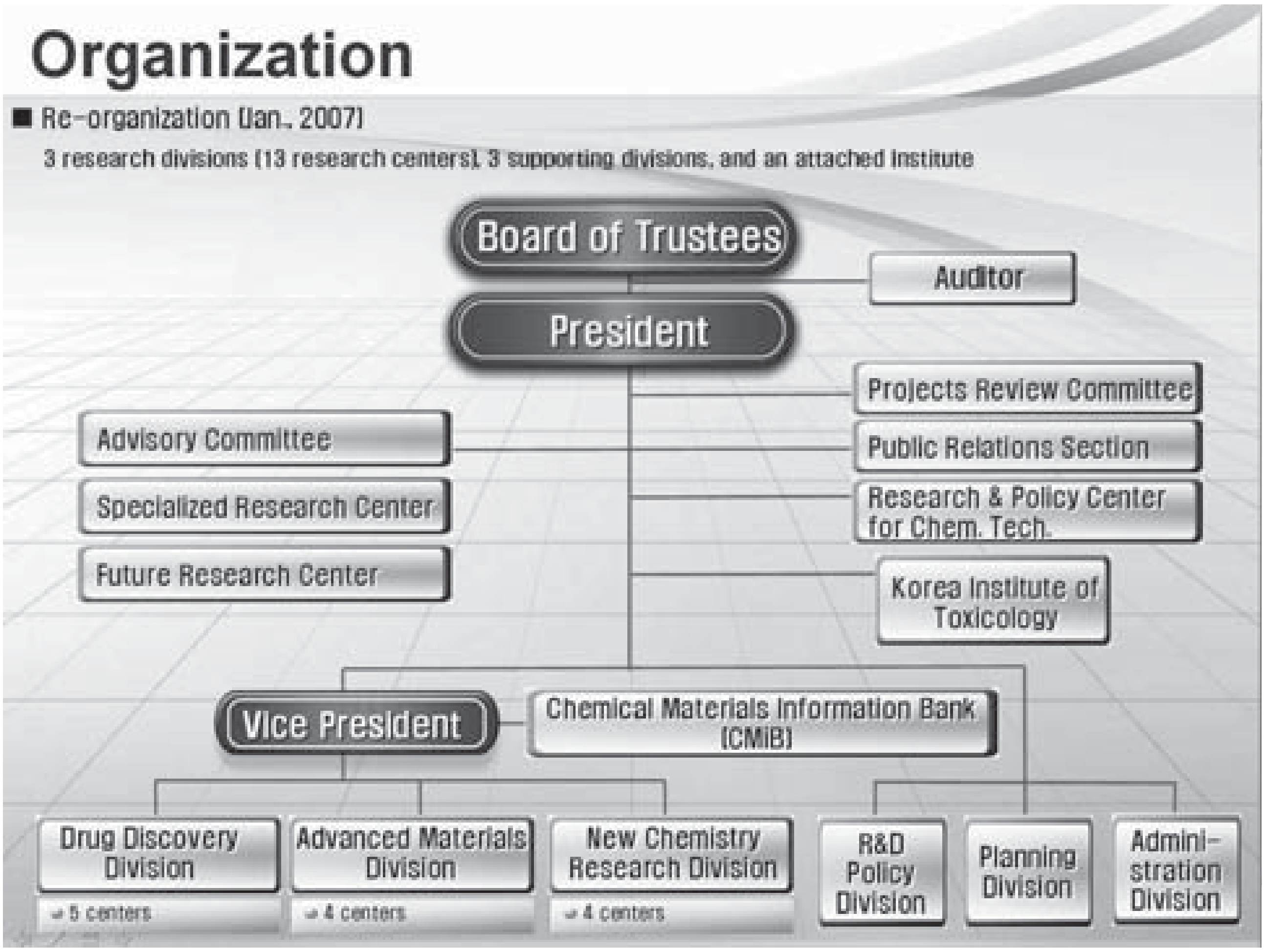

Database Structure
Simulation
Descriptors
Computation (QSPR)
Simulated Properties
Prediction
Verification
Chemical Materials DB
Basic DB
Nomenclature
Chemical Structure
Polymerization DB
Properties DB
Physical Properties
Thermal Properties
Electrical Properties
Monomer DB
Application DB
Toxicology
Reliability
Processing
Spectra DB
NMR, IR
Data Collection
Literature Survey
Basic Properties
Polymerization
Monomer
Industrial Products
Chemical Structure
Polymerization
Processing
DB Collaboration
NIMS, NIST, AIST
Verification of Properties
Data Generation
Basic Properties
Physical Properties
Thermal Properties
Electrical Properties
Application Properties
Toxicology
Reliability
Processing
Spectra
NMR
IR


Chemical Materials Database
Thermolplastic polymer
Thermoset polymer
Rubber & Elastomer
Fine chemical
50 polymer groups
10 polymer groups
40 companies
20 companies
4 companies
20 companies
Total 60 companies
3,300 grades
1,600 grades
300 grades
1,500 grades
4,900 polymer grades
Total ca. 6,700 grades

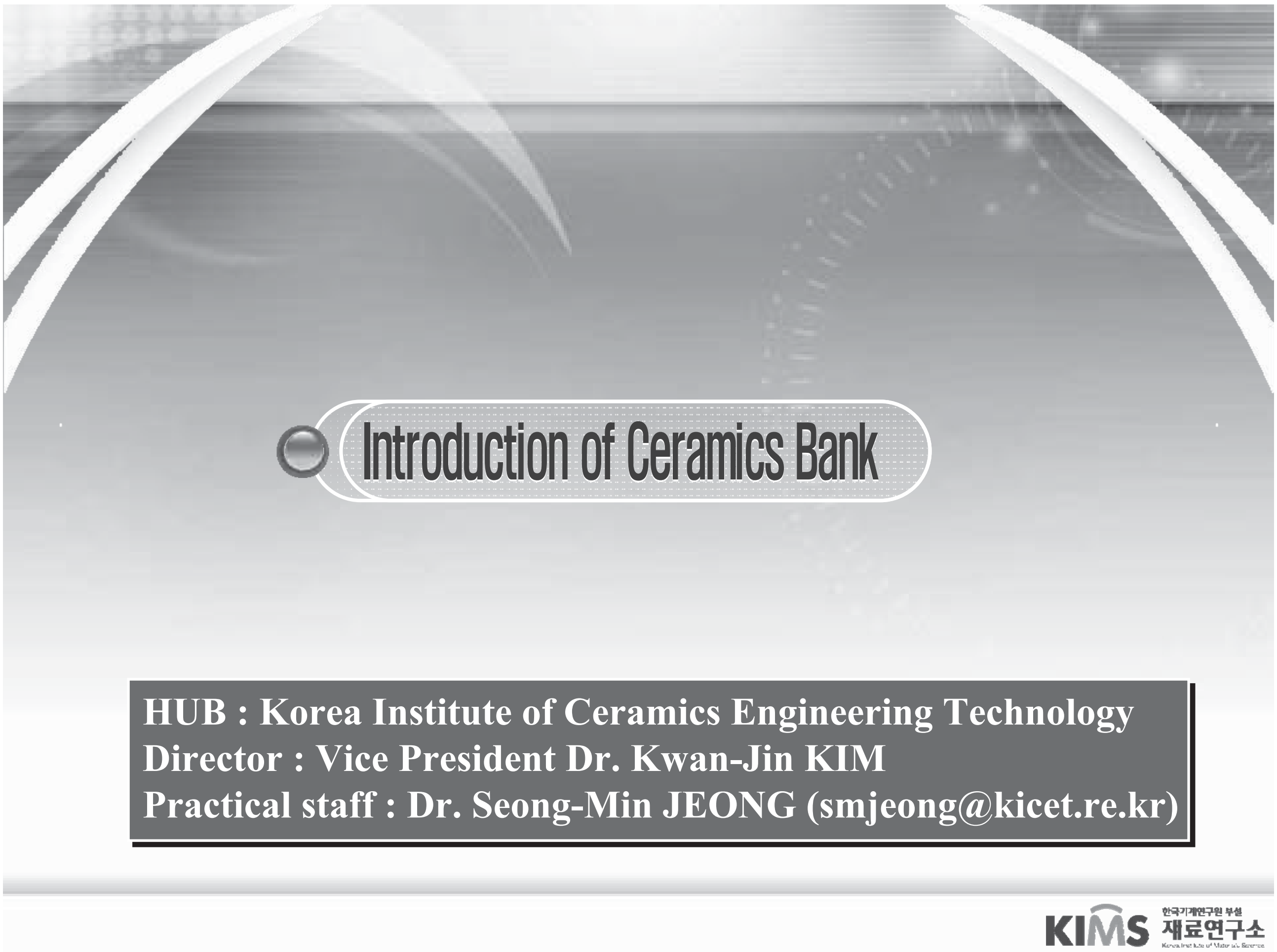

Examples of Polymer Database
Commercial Polymers
Polyolefin
Polymer groups
Types
Code
PE
LDPE
AA
HDPE
AB
Etc.
AZ
PP
Homo-PP
BA
Block-PP
BB
etc.
BZ
Compounded P
BZ
ABS
Polymer groups
Types
Code
ABS
ABS
EA
etc.
EZ
New1
Polymer groups
Types
New code
New1
New1
PA
etc.
PZ
New Polymers
Literature
Academic papers,
Patents, Reports
New polymers are classified by its chemical structures
ZA-ZY
When it is commercially available
Types
code
Types
code
LCP
ZA
PES
ZY
New1
ZZ
New2
ZZ


Introduction of KRICT
KIMS
재료연구소


Location and History
Location
Seoul
Daejeon
Busan
Jeju
KRICT
History
KRICT
1976. 9. Established
- National industry policy
- Self-funding
1980. Growth
- Improved technologies
- Adopting the new technologies
1990. Development
- Long-term national project (G7)
2000. Change
- KIT was established (January.2002)
2006. New take-off
- Three focused research divisions
- Fusion tech.
- 30-years old Anniversary


Organization
■ Re-organization (Jan., 2007)
3 research divisions (13 research centers), 3 supporting divisions, and an attached institute
Board of Trustees
Auditor
President
Projects Review Committee
Advisory Committee
Public Relations Section
Specialized Research Center
Research & Policy Center for Chem. Tech.
Future Research Center
Korea Institute of Toxicology
Vice President
Chemical Materials Information Bank (CMIB)
Drug Discovery Division
5 centers
Advanced Materials Division
4 centers
New Chemistry Research Division
4 centers
R&D Policy Division
Planning Division
Admini-stration Division

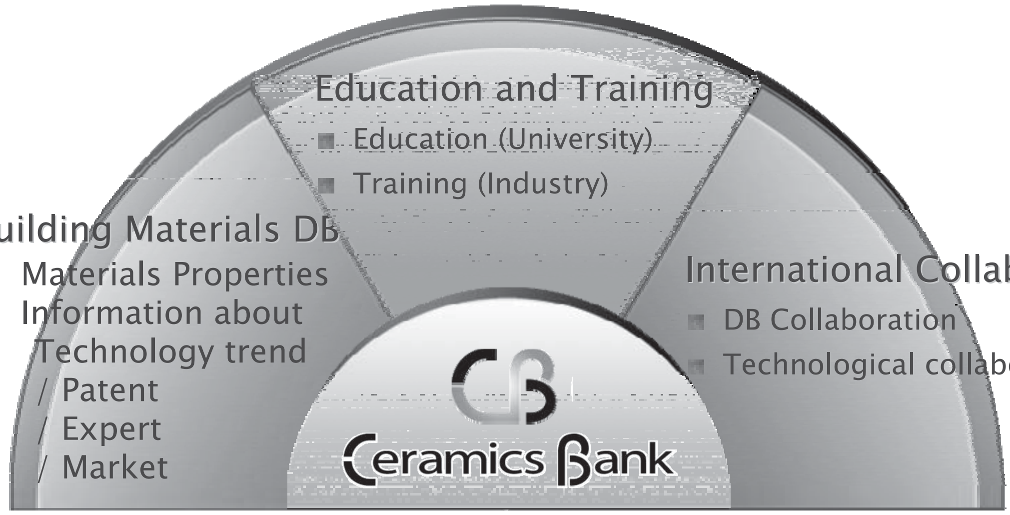

Research Areas
Research Areas : Drug Discovery, Adv. Materials, Sustainable Technology
- From small project-based system to large research centers
Hub of Chemical R&BD for the Industry-Academy-Institution Cooperation
Projects
Drug Discovery Division
Anticancer Drugs
Metabolic Diseases Drugs
Infectious Diseases Drugs
Cardiovascular Diseases Drugs
Advanced Materials Division
Electronic Materials
Display Materials
Bio Sensor Materials
Energy Conversion Materials
New Chemistry Research Division
Green Chemistry & Processes
Utilization Technologies of Petroleum
Bio-Chemical Technologies
Biorefinery Technologies
Supporting Centers
Drug Discovery Research Hub
Chemical Banks
High-throughput Synthesis Center
High-throughput Screening Center
Chemical Materials Information Bank
Information Bank on Chemical Materials
Center for Printable Electronics
Center for Modeling/Simulation of Materials
Supporting Agent for MOCIE on Chemical Processes & Materials
Center for Nanocatalyst
Planning Group for MOCIE Projects
Center for White Biotechnology


Introduction of Ceramics Bank
HUB : Korea Institute of Ceramics Engineering Technology
Director : Vice President Dr. Kwan-Jin KIM
Practical staff : Dr. Seong-Min JEONG (smjeong@kicet.re.kr)
KIMS 재료연구소

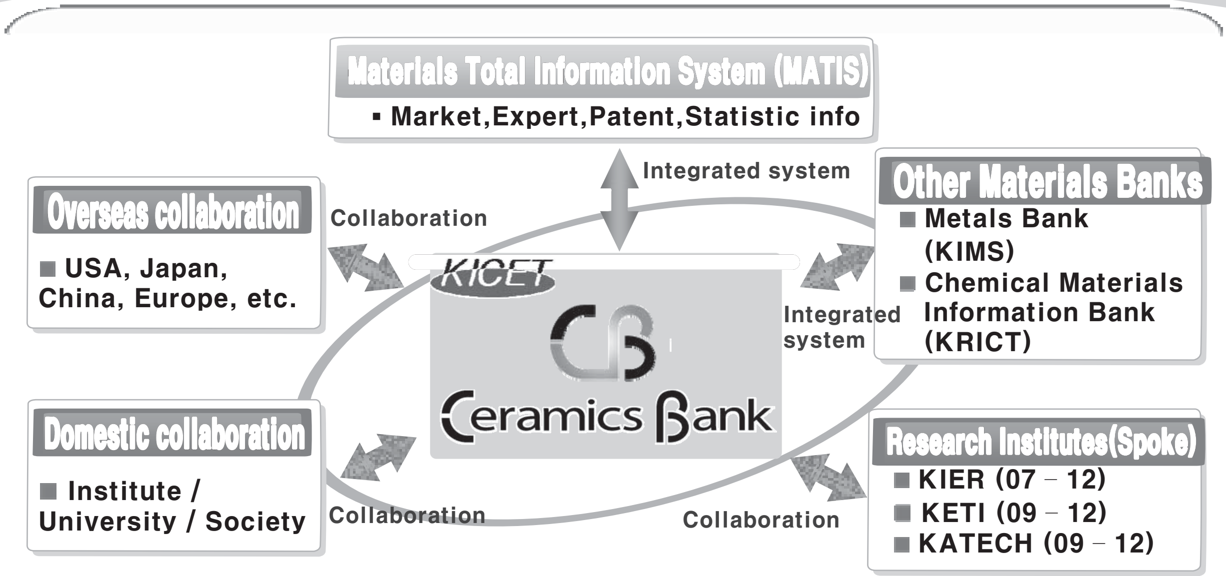
Ceramics Bank Project

◆ Ceramics Bank Project is composed of 3 sections :

- Building Materials Database
- Education and Training
- International Collaboration



Interconnections & collaborations

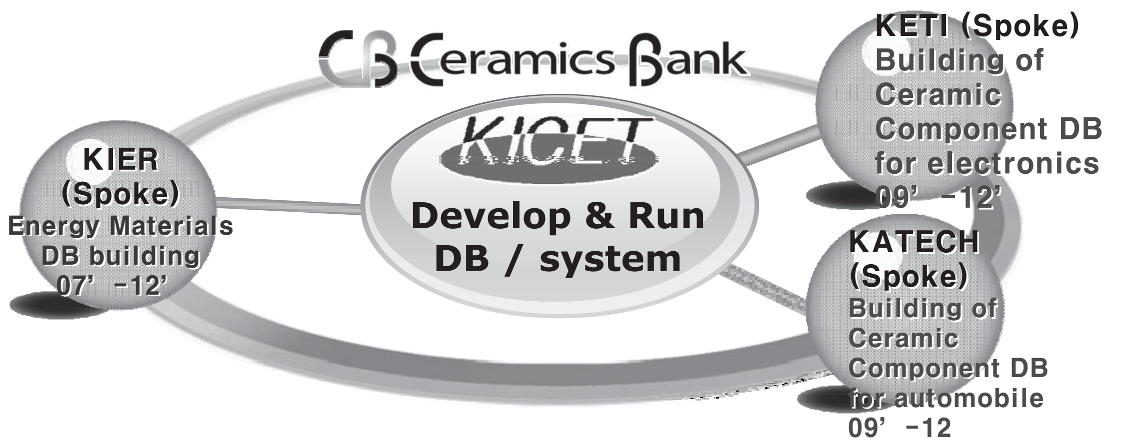


KICET is now activating Ceramic Bank cooperation with other organizations.

Hub and Spoke system

Building Materials Database

Cooperataion between specialized institutes

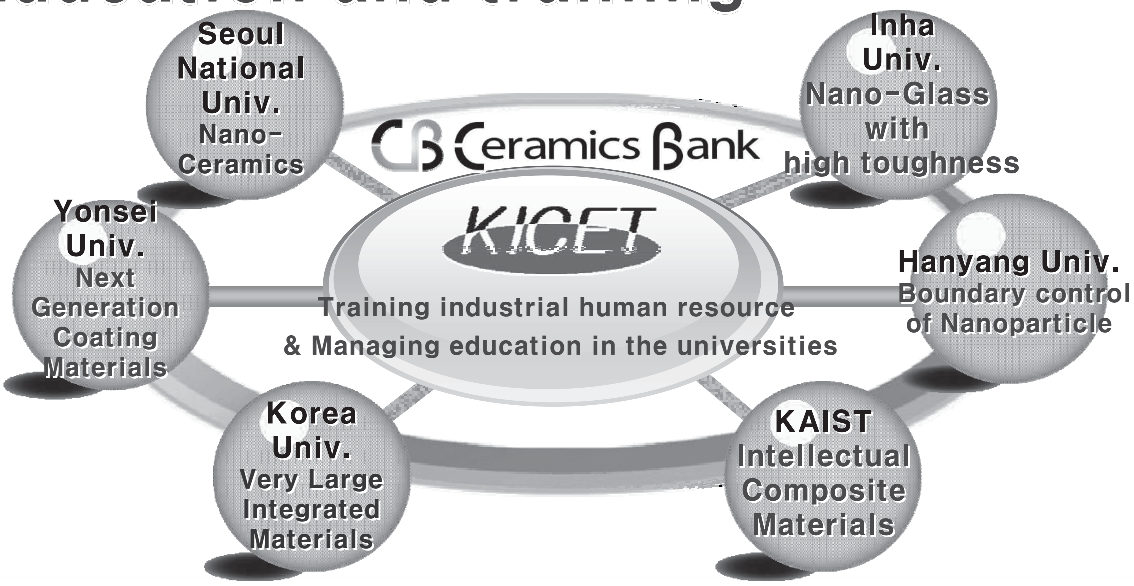


Over than 30 researchers in KICET are currently working to build “Ceramics Bank”.

Ceramics Bank

Hub and Spoke system

Education and training



Hub and Spoke system is also valid for educating and training human resources.

Ceramics Bank

System building

Benchmarking

⇓

Logical modeling

⇓

Data gathering

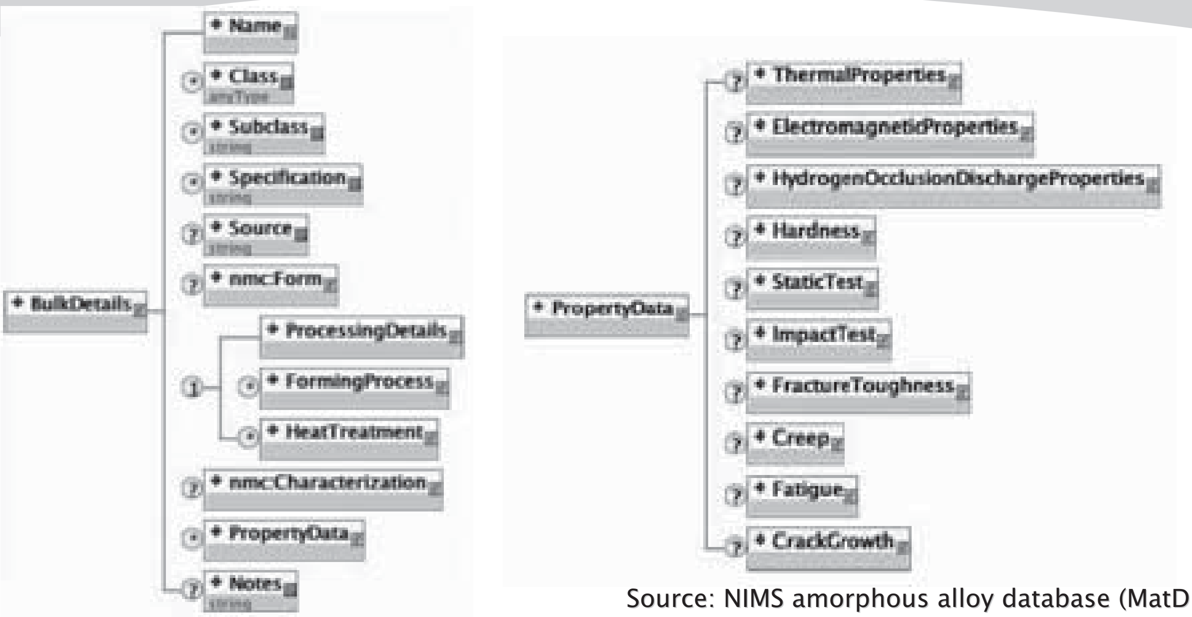
⇓

System design (H/W, S/W)

⇓

Programming

Logical Modeling with XML



Source: NIMS amorphous alloy database (MatDB)

MatML – XML specialized for materials data – make it easy to manage the materials data structure.

Data gathering

Materials Properties

Classification (Application)

Category	No	Class
Electronic	1	Dielectrics
	2	Piezoelectrics
	3	Semiconductor
	4	Conductor
	5	Magnetics
Structural	6	High strength
	7	Injection molding
	8	Non-oxide structural
	9	Porous
Energy / Environmental	10	Functional Catalyst
	11	Air cleansing
Bio	12	Bio (Plate)
	13	Bio
Optical	14	Glass
	15	Coating
	16	Coloring
Analysis		Microstructure
		Chemical

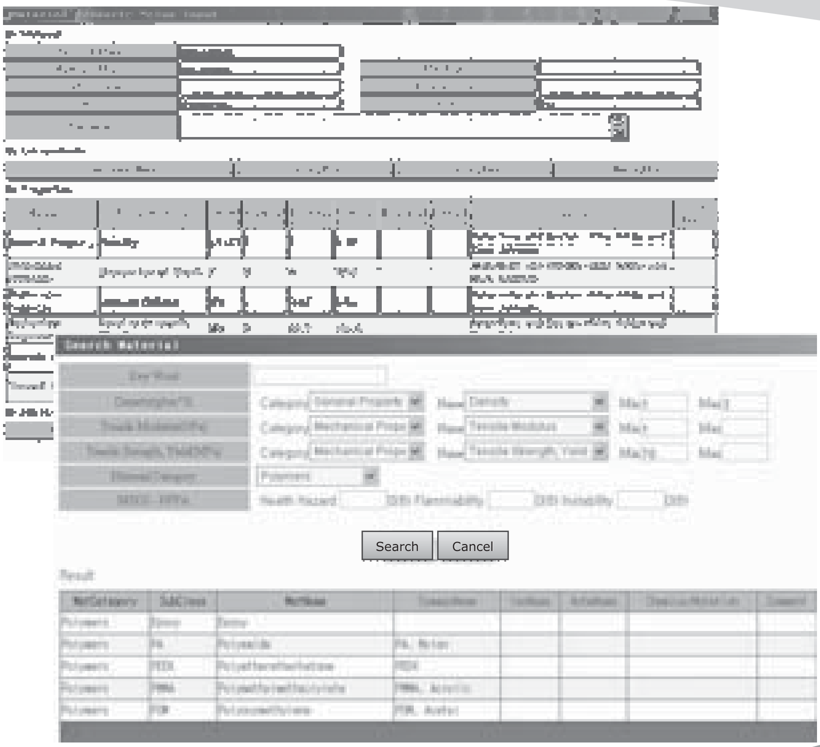
Classification (Data source)

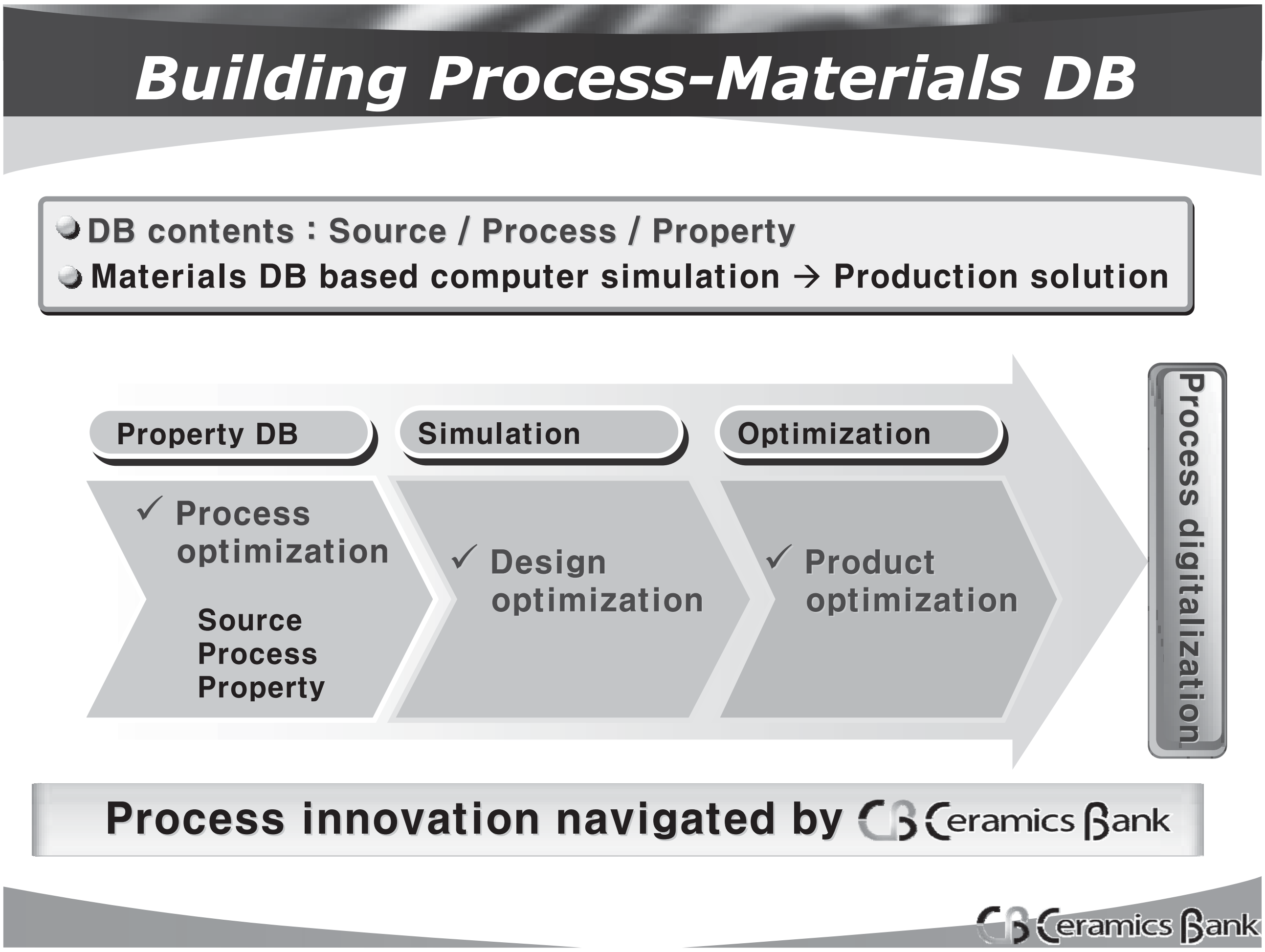
	Data acquisition	Data collection
Category	Materials for : Flat display/ Mobile → Mechatronics → Bio → Clean energy	General information

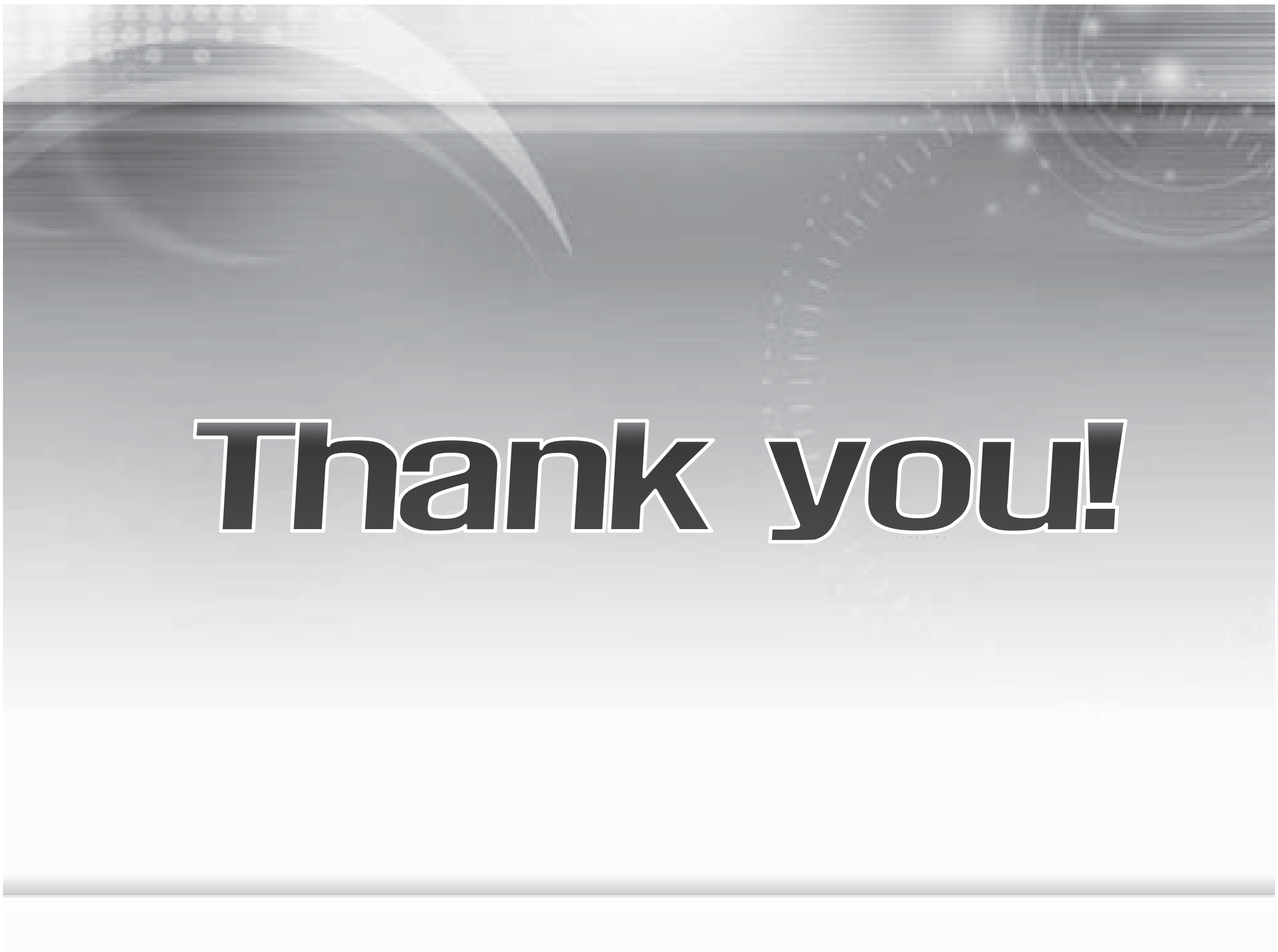
Programming

❖ Search Page
- Search condition input page
- Result page

❖ Characteristics
- Various conditions
  - Key word
  - Up to 3 ranges of properties
  - Material family limitation
  - NFPA
- Result
  - Material List suitable for the condition
  - Detail Result for all properties




Building Process-Materials DB
DB contents : Source / Process / Property
Materials DB based computer simulation → Production solution
Property DB
Simulation
Optimization
✓ Process optimization
Source
Process
Property
✓ Design optimization
✓ Product optimization
Process digitalization
Process innovation navigated by Ceramics Bank
Ceramics Bank


Thank you!

"Construction of Materials Databases and Their Useful Application in the Society of Materials Science, Japan (JSMS)"

Tatsuo SAKAI;

College of Science and Engineering, Ritsumeikan University,
1-1-1 Nojihigashi, Kusatsu, Shiga, 525-8577 Japan

Key words: Fatigue, Database, Statistical analysis, Steel, Aluminum alloy, Solder, *S-N* curve, *P-S-N* curves, Heat treatment, Regression model

Abstract

As a joint project of committees on fatigue of materials and reliability engineering in the Society of Materials Science, Japan(JSMS), fatigue test data for structural metallic materials had been collected in nation-wide scale in Japan and the first databases in both types of databook and machine-readable database were published in 1982. New data obtained after the first publication were also collected and they had been published as the serial databook and database in 1992 by the JSMS. The unit system of CGS was used in the former project, whereas the SI unit was accepted in the latter project. In order to solve this difficulty, all the data compiled in both publications were fully revised as a combined databook and database. Such a new version of the databook was published in the international market in 1996 as a common project of Elsevier and JSMS. But, the machine-readable database has been widely used only in Japan during a long period until now.

In accordance with a progress of the information technology, requirements to the materials database were markedly increased in the latest decades. Thus, JSMS had organized some other projects to construct two different kinds of databases in the area of materials science. The first one is the database on tensile strength and low-cycle fatigue properties of solders. The objective materials are Sn-37Pb and Sn-3.5Ag solders, respectively. The second one is the database on the material characteristics such as stress-strain curves and temperature dependence of heat conductivity, specific heat, elongation and Young's modulus. These databases were being circulated as CD-ROM domestically in Japan at the present stage.

Domestic application of the above databases is in the wide variety such as the fundamental reference data for the fatigue design of the mechanical structures in the industrial society, academic use to analyze the fundamental fatigue behavior of metallic materials and so on. Based on these databases, statistical fatigue property can be also analyzed as design data for the reliability assurance of mechanical structures or electronic systems. In addition, The JSMS had establishes the standard regression method of *S-N* curves in 2002. In the process of edition of this JSMS standard, all the fatigue data in the above JSMS database was repeatedly referred in order to reconfirm the applicability of the JSMS standard. This is a concrete example as the practical use of the databases. English version of this standard was also published in 2007 for the sake of international application of this convenient regression method.

In the present lecture, historical review of the database construction projects in the JSMS and their contents are simply introduced together with some examples of the engineering applications performed by some research groups in the JSMS. Making reference to discussions in the present symposium of MITS2008, the author is looking for the effective method to circulate the JSMS databases in the world-wide scale.

Construction of Materials Databases and Their Useful Application in the Society of Materials Science, Japan (JSMS)

Tatsuo SAKAI

College of Science and Engineering, Ritsumeikan University,
1-1-1 Nojihigashi, Kusatsu, Shiga, 525-8577 Japan

Key words: Fatigue, Database, Statistical analysis, Steel, Aluminum alloy, Solder, *S*-*N* curve, *P*-*S*-*N* curves, Heat treatment, Regression model

Abstract

A series of database construction projects carried out by the Society of Materials Science, Japan (JSMS) in the long term are briefly reviewed, and some examples of the useful application of these databases are introduced together with fundamental problems to be solved in the near future. In addition, the JSMS had established a standardized regression method of S-N curves for metallic materials in 2002, based on the reference use of a lot of data compiled in the database. Thus, this standard regression method of S-N curves is also introduced for the sake of convenience.

History of Database Construction Projects in the JSMS

As a joint project of committees on fatigue of materials and reliability engineering in the Society of Materials Science, Japan(JSMS), fatigue test data for structural metallic materials had been collected in nation-wide scale in Japan and the first databases in both types of databook and machine-readable database were published in 1982. This project would be the first attempt to construct the materials database in Japan. Thus, the fundamental concept and format of the database in this project were often referred to the succeeding database construction projects.

New data obtained after the first publication were also collected and they had been published as the serial databook and database in 1992 by the JSMS. The unit system of CGS was used in the former project, whereas the SI unit was accepted in the latter project. In order to solve this difficulty, all the data compiled in both publications were fully revised as a combined databook and database. Such a new version of the databook was published in the international market in 1996 as a common project of Elsevier and JSMS [1]. But, the machine-readable database has been widely used only in Japan during a long period until now.

In accordance with a progress of the information technology, requirements to the materials database were markedly increased in the latest decades. Thus, JSMS had organized some other projects to construct three different kinds of databases in the area of materials science. The first one is the database on fatigue crack growth rates of metallic materials. This was constructed as reference data to assess the safety of mechanical structures having defects such as fatigue cracks. The second one is the database on tensile strength and low-cycle fatigue properties of solders. The objective materials are Sn-37Pb and Sn-3.5Ag solders, respectively. The third one is the database on the material characteristics such as stress-strain curves and temperature dependence of heat conductivity, specific heat, elongation and Young's modulus. These databases were being circulated as CD-ROM domestically in Japan at the present stage.

Contents of Respective Databases in the JSMS

Database on Fatigue Strengths of Metallic Materials

Types of Fatigue Test Data
SN data: Conventional fatigue test data to obtain S-N characteristics
ST data: Fatigue test data obtained by staircase method
PN data: Fatigue test data to obtain fatigue life distribution characteristics
and fundamental data such as
Name of material, chemical composition, heat treatment conditions, mechanical properties, shape and dimensions of specimen, fatigue testing conditions
are compiled for each test series of the respective metallic materials. All the data are compiled in both electronic database and databooks of 3 volumes, in which S-N diagrams and the fatigue life distribution curves are also printed.

The Number of Data Series

< *Ferrous Metals* >

Steels for machine structural use:	275 series
Steels for automobile structural use:	47 series
Steels for special purpose use:	59 series
Carbon steels and alloy steels:	1,533 series
Stainless steels and heat resistant steels:	366 series
Cast irons, cast steels, etc.:	351 series
Total	2,631 series

< *Non-ferrous Metals* >

Copper and copper alloys:	42 series
Aluminum and aluminum alloys:	215 series
Aluminum and copper castings:	69 series
Magnesium alloys:	5 series
Titanium alloys:	33 series
Silver alloy:	1 series
Zn alloys:	1 series
Powder metallurgy:	50 series
Total	416 series
Grand total (Ferrous + non-ferrous metals)	3,047 series

Database on Fatigue Crack Growth Rates of Metallic Materials

Experimental data on fatigue crack growth rates for many kinds of metallic materials are compiled together with fundamental data such as name of material, chemical composition, heat treatment conditions, mechanical properties, shape and dimensions of specimen, fatigue testing conditions. The format of the fundamental data is quite same as that in the former database on fatigue strength of metallic materials. In this case, a type of databook was also published consisting of a pair of pages, in one of which numerical data are printed and in the other page $da/dN - \Delta K$ diagram (Paris Law) is depicted with parameters in the crack growth law.

This database can be usefully referred to evaluate the safe fatigue life of structural components having a certain length of cracks, since one can analyze the crack propagation life from the initial length to the critical length to occur the final fracture.

Database on Tensile Strength and Low-cycle Fatigue Properties of Solders

The objective materials are Sn-37Pb and Sn-3.5Ag solders, respectively. The standard testing method of the tensile test for solders had established and the JSMS standard [JSMS-SD-2-00] was published in 2000. At that time, another standard testing method of low cycle fatigue for solders was also published by the society of JSMS as a pair of publications. Thus, the JSMS Committee on High Temperature Strength of Metallic Materials had organized a series of round robin tests on tensile test and low cycle fatigue test for the above two kinds of solders. The present database was constructed by collecting these testing results obtained by the definite procedure given in the JSMS standards.

Materials Property Database for Heat Treatment Simulation

Experimental data such as CCT-property, TTT-property, heat conductivity, specific heat, thermal expansion, S-S curve and so on are collected and compiled as machine readable database by a committee in the JSMS. This database can be usefully applied to make simulations for heat treatments such as quenching and tempering for structural steels. In the process of these heat treatments, temperature dependence of the respective material properties plays an important role to give the final mechanical properties. Thus, the present database was constructed paying a particular attention to the temperature dependence of the respective properties.

Softwares to Extract and Analyze the Materials Databases in the JSMS

Service media in the series of materials databases published by the JSMS is either type of floppy disc, CD-ROM or cassette tape, respectively. At the present stage, every database has been provided to users in any type of the above media without any internet service through the web-site. Thus, software to extract the required data should be prepared by individual users, and the user should develop the software to analyze the database depending on the respective purposes of the database applications.

In such a circumstance, many companies have been developing a lot of kinds of softwares to extract and analyze the materials databases including the JSMS databases. For instance, the engineering software of *METIS* developed by Mitsubishi Research Institute, Inc., and the web-based engineering system of the machine design handbook compiled in the *i-engineering* developed by Hitachi Ltd. are typical examples of such engineering applications. In addition, some committees in the JSMS have also developed various kinds of softwares in order to analyze individual articles depending on the respective requirements. These softwares have been used by the respective committees or working groups as the closed uses and applications.

The JSMS Administration Committee on Materials Database is now planning to open JSMS databases for the international service through the internet web system. The first candidate is the database on fatigue strength of metallic materials. Thus, the fundamental functions to extract the required kind of material and to analyze the S-N characteristics for the material should be included in such a system. Fortunately, the JSMS has established the standard regression method of the S-N curve, and the JSMS standard in English version [JSMS-SD-11-07] has been published in 2007 [2]. Since this standard has an important role to facilitate the useful applications of the JSMS database, contents of this standard is a little more explained in later.

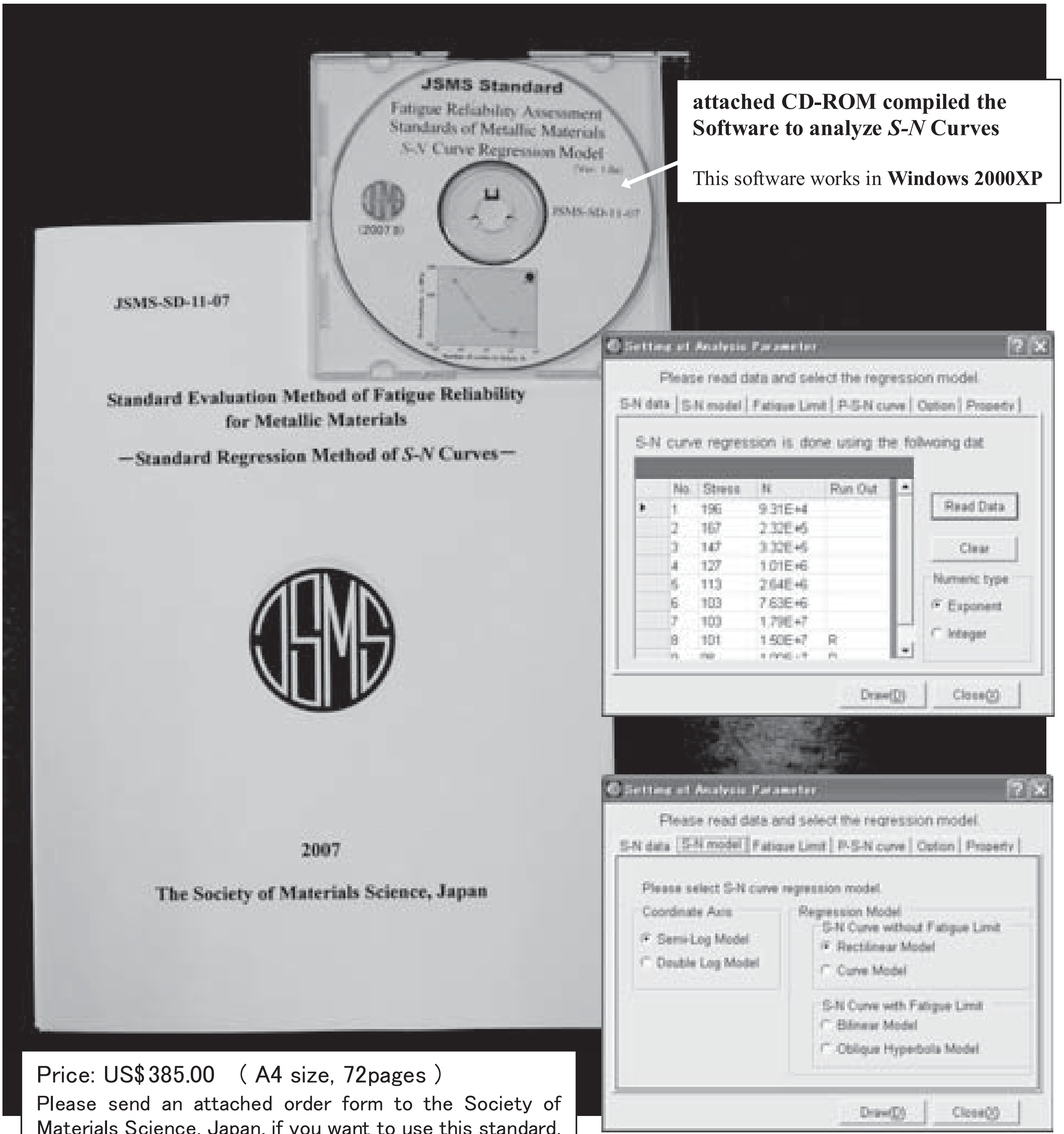
Standard Regression Method of S-N Curves

Leaflet of the JSMS standard published in 2007 is provided in the following four pages, in which some examples of S-N curves and P-S-N curves analyzed by this standard regression method are also attached for the sake of convenience.

Standard Evaluation Method of Fatigue Reliability
for Metallic Materials
- Standard Regression Method of *S*-*N* Curves -
[JSMS-SD-11-07]

published by

the Society of Materials Science, Japan
1-101 Yoshida Izumidono-cho, Sakyo-ku, Kyoto, 606-8301, Japan



Committee on Standardization of Fatigue Reliability Evaluation of Metallic Materials

Chairman
Tatsuo SAKAI; Ritsumeikan University
Vice-chairman
Atsushi SUGETA; Hiroshima University
Executive Members
Satoshi HANAKI; University of Hyogo
Masaki NAKAJIMA; Toyota National College of Technology
Yuji NAKASONE; Tokyo University of Science
Hidetoshi NAKAYASU; Konan University
Izuru NISHIKAWA; Osaka Institute of Technology
Kenji OKADA; Takamatsu National College of Technology
Hideo ONO; Kawaju Techno Service Corp.
Akiyoshi SAKAIDA; Akashi National College of Technology
Toshio SHUTO; Mitsubishi Research Institute, Inc.
Kazuto TANAKA; Doshisha University
Toshinori YOKOMAKU; Kobelco Research Institute, Inc.
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Hiroshige ITO; Toshiba Corporation
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Saburo MATSUOKA; Kyushu University
Yasuaki OHMI; Toyota Motor Corporation
Nagatoshi OKABE; Ehime University
Takashi SAKAI; Takamatsu National College of Technology
Kazuaki SHIOZAWA; Toyama University
Miyuki YAMAMOTO; Sumitomo Metal Industries, Ltd.

Objective and Scope

Every mechanical structure consists of many components made of various materials primarily of metals. In order to evaluate the fatigue reliability of a mechanical structure, it is necessary to verify fatigue characteristics of the structural materials. In the test method generally used to examine such fatigue characteristics of metallic materials, the stress ratio R or the mean stress σ_m is kept constant and different cyclic stress is applied to each test piece by changing the stress amplitude σ_a, where the number of stress cycles to failure is obtained as the fatigue life N. Based on such experimental results, the fatigue property is usually represented as "*S-N* curve". Aim of the present "Standard Evaluation Method of Fatigue Reliability for Metallic Materials; -Standard Regression Method of *S-N* curves-" (hereafter "the Society's Standard") is to provide the standard procedure for statistical regression of the *S-N* curve based on fatigue test data.

For the *S-N* property of metallic materials, fatigue behavior at higher stress range with relatively short fatigue life is different from that at lower stress range with relatively long fatigue life. Therefore, they have been classified into different categories of *"Low Cycle Fatigue"* and *"High Cycle Fatigue"*. In addition, some unique fatigue characteristics of metallic materials in the ultra-long life regime such as gigacycle or higher have been recently reported as *"Very High Cycle Fatigue"* by many researchers. Thus, the fatigue characteristics vary among different life ranges. The fatigue life cycles discussed in the Society's Standard is limited to the fatigue life regime conventionally so-called *"High Cycle Fatigue"*. Therefore, fatigue characteristics in the low cycle regime and the ultra-long life regime are not included in the analysis.

S-N Curve Regression Models

_S-N_ curve with fatigue limit

For the type of *S-N* curve with fatigue limit, only the bilinear folded line and the oblique hyperbola curve are adopted and both of semi-logarithmic coordinates and double logarithmic coordinates are introduced to represent the *S-N* curves. The stress amplitude is hereafter expressed by σ for the sake of simplicity.

1) Bilinear regression model

(1) Semi-logarithmic bilinear model

$$\sigma = -A\log_{10} N + B \ (N < N_w),\ \sigma = E \ (N \geq N_w)$$

(2) Double logarithmic bilinear model

$$\log_{10} \sigma = -A\log_{10} N + B \quad (N < N_w),$$
$$\log_{10} \sigma = \log_{10} E \quad (N \geq N_w)$$

where A, B, E and N_w are constants.

2) Curve regression model

(1) Semi-logarithmic oblique hyperbola model

$$(\sigma - E)\ (\sigma + A\log_{10} N - B) = C$$

(2) Double logarithmic oblique hyperbola model

$$(\log_{10} \sigma - \log_{10} E)\ (\log_{10} \sigma + A\log_{10} N - B) = C$$

where $A, B, C,$ and E are constants.

_S-N_ curve without fatigue limit

For the type of *S-N* curve without fatigue limit, the straight line and the curved line are adopted to represent the *S-N* curves by using both of semi-logarithmic coordinates and double logarithmic coordinates. Even for ferrous metals which exhibit clear fatigue limits, the *S-N* curve without fatigue limit is assumed referring to the finite life range, if experimental results only on the slope portion of an *S-N* curve are available without any run-out datum.

1) Rectilinear regression model

(1) Semi-logarithmic rectilinear model

$$\sigma = -A\log_{10} N + B$$

(2) Double logarithmic rectilinear model

$$\log_{10} \sigma = -A\log_{10} N + B$$

where A and B are constants.

2) Curve regression model

Curve regression model for the *S-N* curve without fatigue limit is fundamentally based on Stromeyer's expression, $\log_{10} (\sigma - D) = -A \log_{10} N + B$, and it is rewritten into a regression model of Expression (7) in semi-logarithmic coordinates, and that of Expression (8) using the double logarithmic coordinates.

(1) Semi-logarithmic curve model

$$\sigma = 10^{-A \log 10\, N + B} + D$$

(2) Double logarithmic curve model

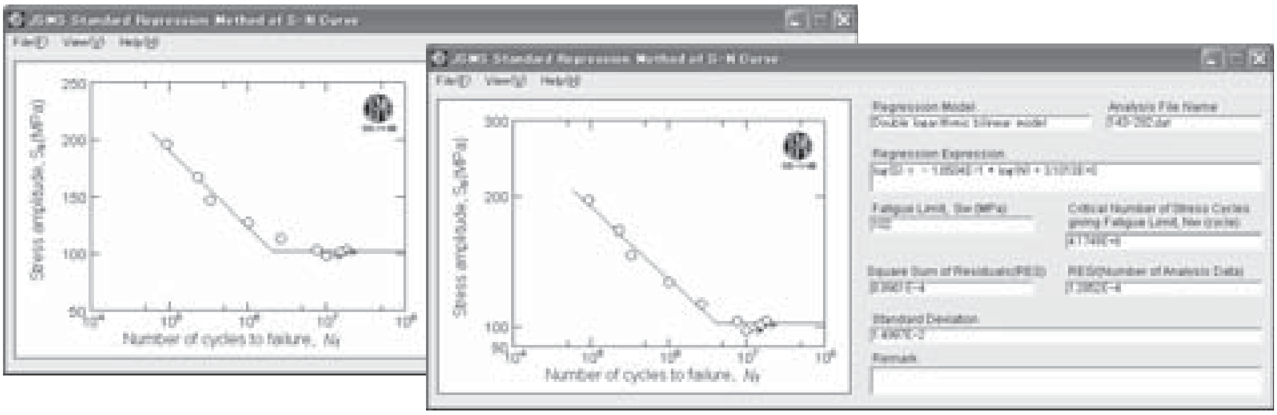
$$\log_{10} \sigma = \log_{10} \ (10^{-A \log 10\, N + B} + D)$$

where A, B, and D are constants.

Analysis Examples of *S-N* curves with fatigue limit (ferrous metals, titanium alloys, etc.)

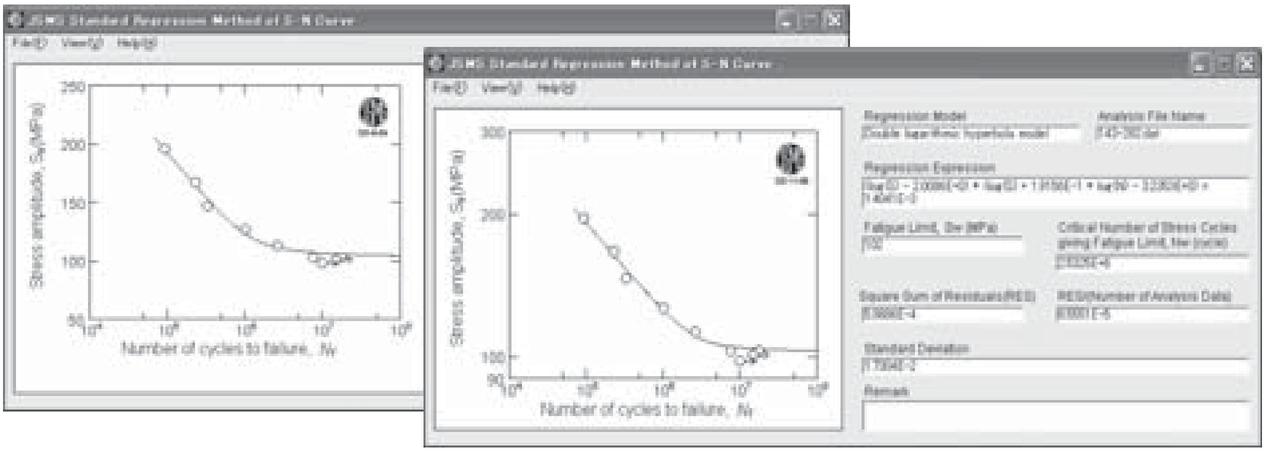
Some typical examples of *S-N* curves with fatigue limit obtained by the present standard regression method are shown in Example1, 2, and 3, respectively.

Example 1(a)　Semi-logarithmic bilinear model (S10C, R=-1)



Example 1(b)　Double-logarithmic bilinear model (S10C, R=-1)

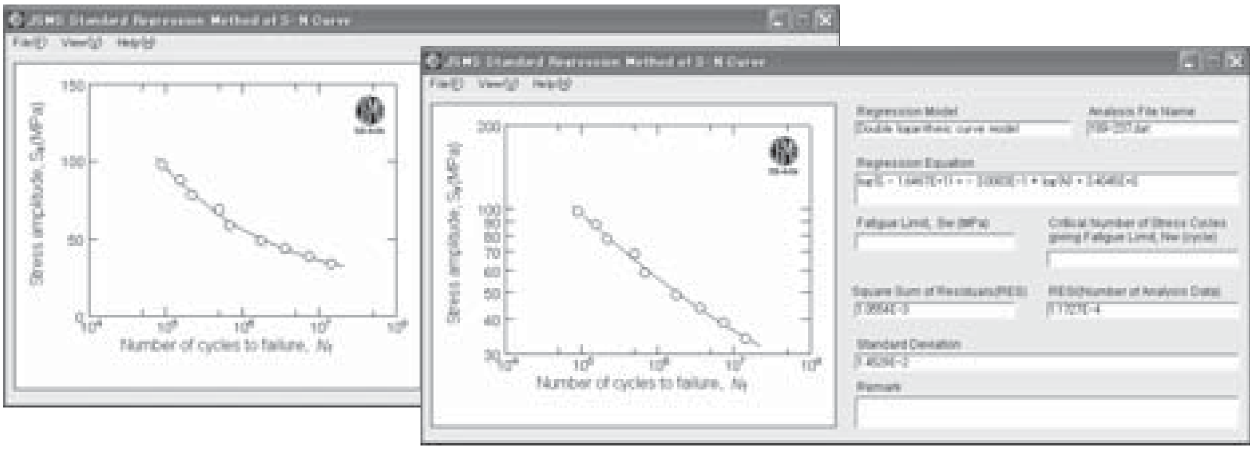
Example 2(a)　Semi-logarithmic oblique hyperbola model (S10C, R=1)



Example 2(b)　Double-logarithmic oblique hyperbola model (S10C, R=1)

Analysis Examples of *S-N* curves without fatigue limit (aluminum alloys, copper alloys, etc.)

Example 3(a) Semi-logarithmic curve model (A7075-T6, *R*=-1)

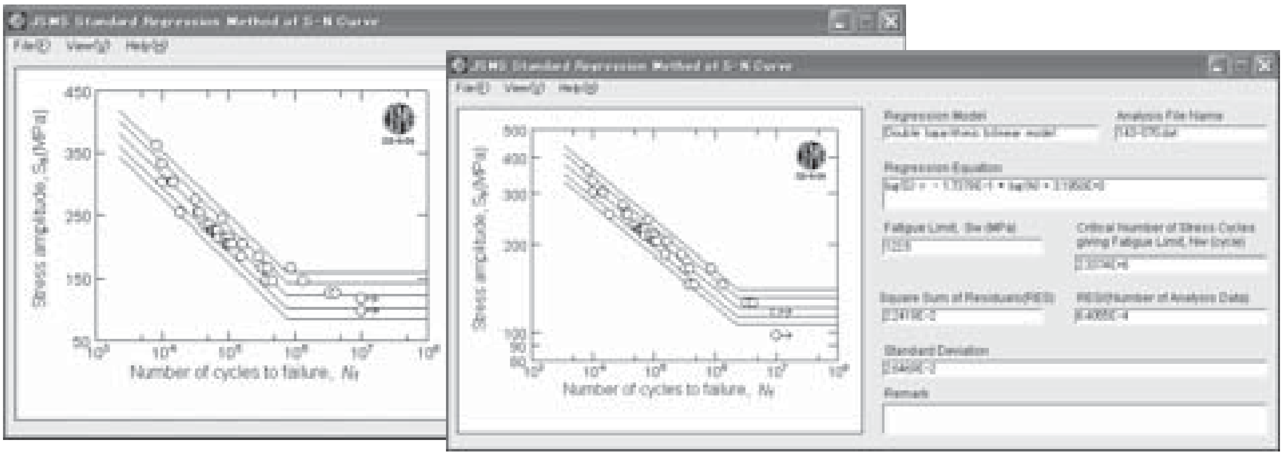


Example 3(b) Double logarithmic curve model (A7075-T6, *R*=-1)

Analysis Examples of *P-S-N* curves with fatigue limit (ferrous metals, titanium alloys, etc.)

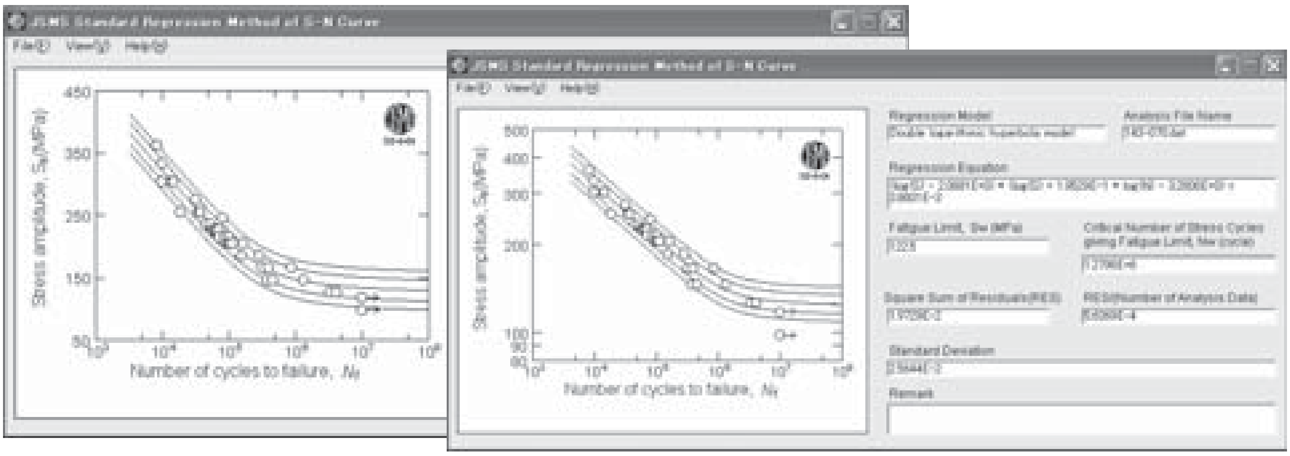
A group of 5 curves in each drawing indicate *P-S-N* curves with the probabilities of failure of 1%, 10%, 50%, 90%, and 99%, from left (bottom) in order respectively.

Example 4 (a) *P-S-N* curves in semi-logarithmic bilinear model (S10C, *R*=-1)



Example 4 (b) *P-S-N* curves in double logarithmic bilinear model (S10C, *R*=-1)

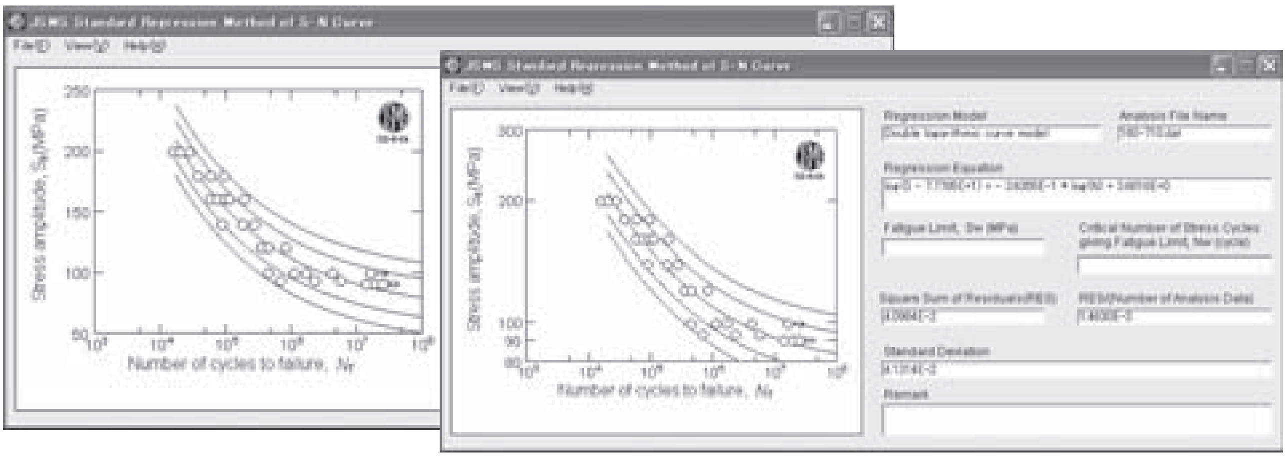
Example 5 (a) *P-S-N* curves in semi-logarithmic oblique hyperbola model (S10C, *R*=-1)



Example 5 (b) *P-S-N* curves in double logarithmic oblique hyperbola model (S10C, *R*=-1)

Analysis examples of *P-S-N* curves without fatigue limit (aluminum alloys, copper alloys, etc)

Example 6 (a) *P-S-N* curves in semi-logarithmic curve model (JIS AC8B, *R*=-1)



Example 6 (b) *P-S-N* curves in double logarithmic curve model (JIS AC8B, *R*=-1)

Applications of Materials Database to Analyze the Statistical Fatigue Property

A lot of fatigue test data are required to analyze the fatigue characteristics of metallic materials. But, such a kind of the fatigue data are not always provided in advance. On the other hand, conventional fatigue test data to obtain the S-N property have been reported and filed for many kinds of metallic materials. If one can pool these usual S-N data altogether based on a certain normalization, the statistical fatigue property can be analyzed effectively from the pooled data.

As an example, S-N data for low carbon steels of S10C were extracted from the JSMS database on the fatigue strength of metallic materials [2], and they were plotted as S-N diagram in Fig.1. Total number of data series for S10C steel is 46 and total number of data points is 1161. In addition, 4 series of fatigue test data with 67 data points in total for pure iron are included in the JSMS database. Thus, these data points are plotted by marks of triangles. Even if the material is limited for S10C steel, carbon contents are in a certain range of scatter and the strength level has the corresponding scatter. Accordingly, fatigue strength has also some scatter as indicated in Fig.1. Since the strength level of the pure iron is lower than that for S10C steel, their fatigue data are plotted along the lower bound in the S-N property in Fig.1.

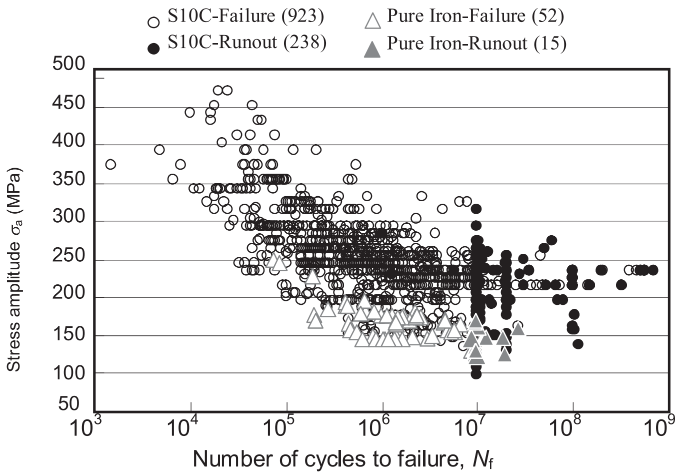


Fig.1 $\sigma_a - N$ diagram plotted all data on S10C and Pure Iron

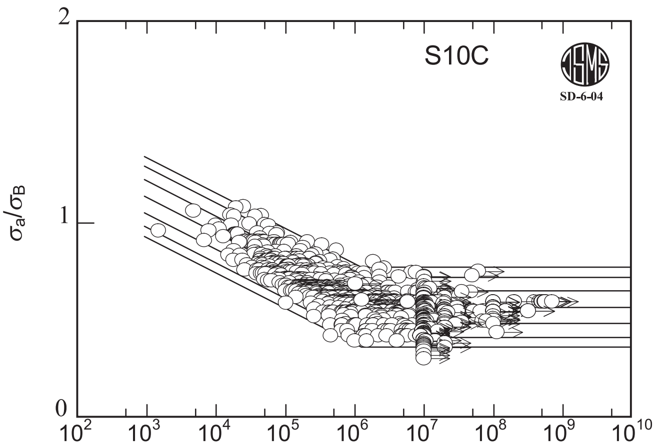


Fig.2 $\sigma_a/\sigma_B - N$ diagram(Bilinear regression model)

In this place, normalizing the applied stress by the tensile strength of each series of S10C specimens, all the S-N data are again plotted in Fig.2. It is found that all the fatigue data tend to appear within a common scatter range in Fig.2. Therefore, one can analyze the P-S-N characteristics by applying the standard regression method introduced in the previous section. P-S-N curves giving failure probabilities of 0.1%, 1%, 10%, 50%, 90%, 99% and 99.95, respectively are indicated in Fig.2 [3].

Let us similarly replot the fatigue test data for the pure irons together with those for the S10C specimens in Fig.3. Thus, one can find that the data for the pure irons are yielding along the central position of the whole data points in Fig. This fact suggests us that the low carbon steel of S10C and the pure iron can be successfully pooled as common population data for statistical fatigue characteristics. Based on this evidence, one can similarly analyze the statistical fatigue property for such a common population as P-S-N characteristics by using the JSMS standard of the S-N curve regression [2].

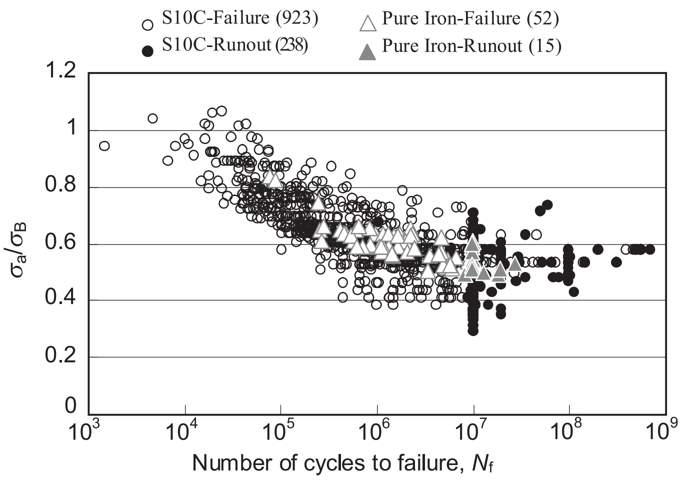


Fig.3 σ_a/σ_B-N diagram (plotted all data on S10C and Pure Iron)

In order to reconfirm this aspect, fatigue test data for carbon steel of S45C with medium level of carbon contents were extracted from the above JSMS database. After the applied stress was normalized by the tensile strength, those data were plotted as S-N diagram in Fig.4. Since all the data points thus normalized are appearing along a common scatter band, one can similarly analyze the P-S-N characteristics as indicated in Fig.4.

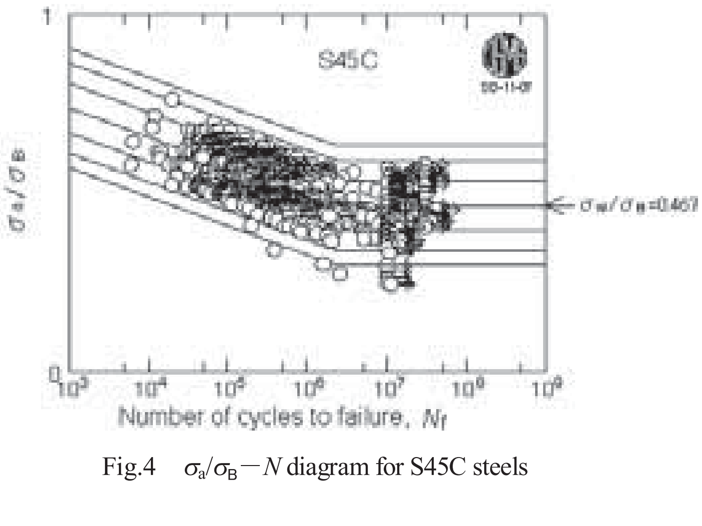


Fig.4 σ_a/σ_B-N diagram for S45C steels

Concluding Remarks

In this presentation, a series of materials databases constructed and published by the society of JSMS were briefly introduced. And, some useful applications of the JSMS database on fatigue strength of metallic materials were shown in this report as concrete examples in an area of the reliability engineering.

Every kind of the database should be expanded by collecting newly obtained experimental data and error corrections should be made at every chance whenever any error was found. Such a maintenance for the materials database is fundamentally important, but it is not so easy to keep the high quality of every database. From the long term experience of the author in this area, the most important articles to maintain the database are pointed out as follows;

(1) Elaborated design of the fundamental format
(2) Simplification and efficiency of data input system
(3) Sufficient quantity of compiled data (All the data under definite conditions should be collected)
(4) Correctness of all the compiled data
(5) A standing project team for data collection and their debugging

In addition, financial background of the database project should be firmly investigated and discussed in advance. Initial cost of the database project is usually very high and another cost to maintain the database is also not so cheap during a long period without the final life. At some stages in the last decades, some kinds of social fund were often provided into the database construction projects in every country including Japan. However, a kind of financial difficulty is taking place as a common problem. A common trend that a definite project team cannot be kept during a long term brings us another difficulty to facilitate the database project for the sake of the society's convenience.

In accordance with the progress of the Information Technology, requirement to the materials database is supposed to be accelerated in various areas of the industrial societies. In such a circumstance, the author is supposing that only following two types of material databases can have the steady position in the future society beyond the present century;

(1) Material databases financially supported by some kinds of public funds

In this case, the database project itself should be approved as a public long-span project. But, a strict difficulty is supposed, since the government of each country or each domestic area is usually limited in the foundation.

(2) Material databases commercially sustainable for definite societies

Balance of *consumption* and *supply* is fundamentally important even for the material databases. If sufficient survey was performed in advance and some size of steady customers was expected, one should estimate the costs of database construction and maintenance carefully. If a commercial sustainability is firmly convinced, then one can organize the database project. This is the most natural aspect for every project required some amount of financial fund. The most important point is that every database should be constructed by focusing the concrete costomers.

References

1) K. Shiozawa, T. Sakai et al., *Databook on Fatigue Strength of Metallic Materials,* Vols.1-3, (1996), Elsevier and JSMS.
2) T. Sakai et al., *Standard Evaluation Method of Fatigue Reliability for Metallic Materials, - Standard Regression Method of S-N Curves-,* JSMS-SD-11-07, (2007), JSMS.
3) K. Okada et al., Statistical fatigue properties of ultra low carbon steels under rotating bending based on JSMS database on fatigue strength of metallic materials, *J. Soc. Mat. Sci., Japan,* Vol.56, (2007), p.1170.

Current Status and Future Prospect of Materials Data Sharing in China

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The materials data resource is abundant and there existing a variety of databases which are dispersed, not comprehensive and lack of systematicness in China. National scientific data sharing program was launched to function as a catalyst to integrate scientific data resources and to promote the integration was put forward in National Guidelines for Medium- and Long-term Plans for Science and Technology Development. National materials scientific data sharing project, as a part of National scientific data sharing program, is under construction and covers 8 categories of materials from metal to natural material. Data query system is realized, material database design specification is put forward and a key problem of query over heterogeneous data sources is settled.

Current Status and Future Prospect of Materials Data Sharing in China

Yin Haiqing

with acknowledgements to Qu Xuanhui, Liu Guoquan, Hu Changjun, Li Changrong, Zhao Chongchong, Bao Hong, Xing Lihong

University of Science and Technology Beijing, China

2008.07.18

UNIVERSITY OF SCIENCE AND TECHNOLOGY BEIJING

Outline

1. Brief introduction of University of Science and Technology Beijing (USTB)
2. History of material database in China
3. Current resources of material databases
4. Strategies and policies from government
5. Introduction to National Material scientific data sharing project
6. Summary

UNIVERSITY OF SCIENCE AND TECHNOLOGY BEIJING

1. Brief Introduction of University of Science and Technology Beijing

- **The University of Science and Technology Beijing (USTB), founded in 1952, is a national key university under the direct supervision of the Ministry of Education of China .**

- **USTB is famous for its study in metallurgy and materials science and engineering. It is leading university in these fields in China.**

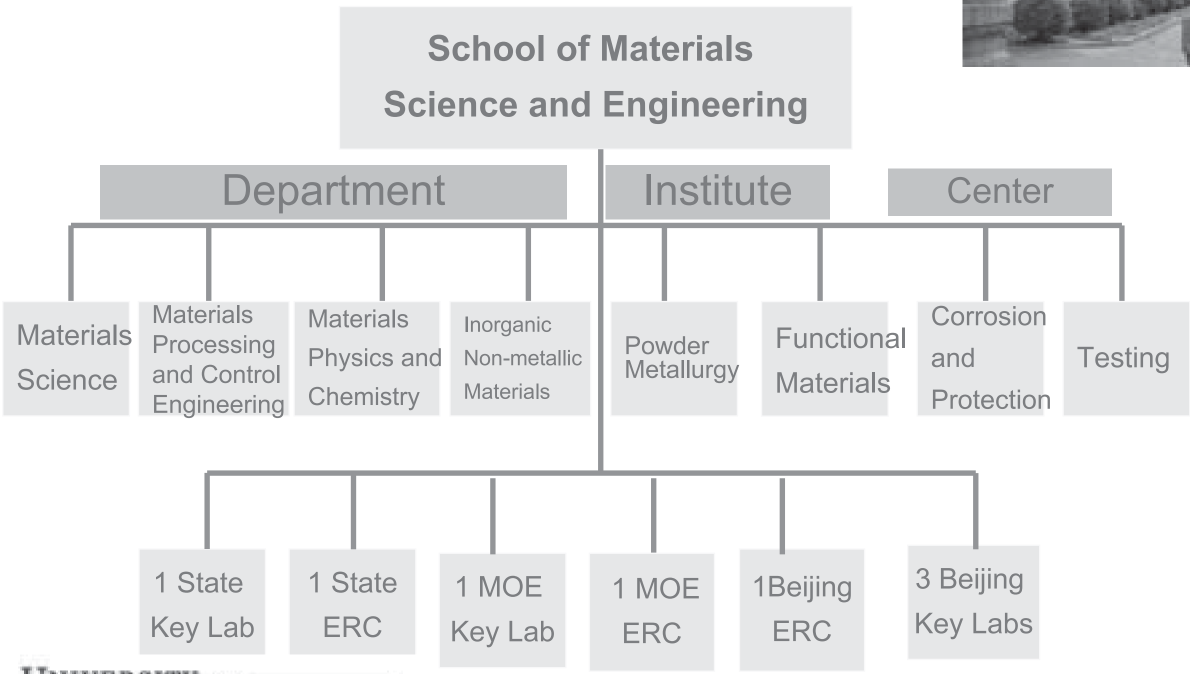
UNIVERSITY OF SCIENCE AND TECHNOLOGY BEIJING

Brief Introduction of USTB

- There are 9 Schools at USTB, covering civil and environmental engineering, information engineering, materials science and engineering, mechanical engineering, metallurgical and ecological engineering, management, applied Science, foreign languages, humanities and social sciences.

- While engineering is the focus, there are also programs in basic science, management, humanities, economics and law.

Organization Structure, since 2001



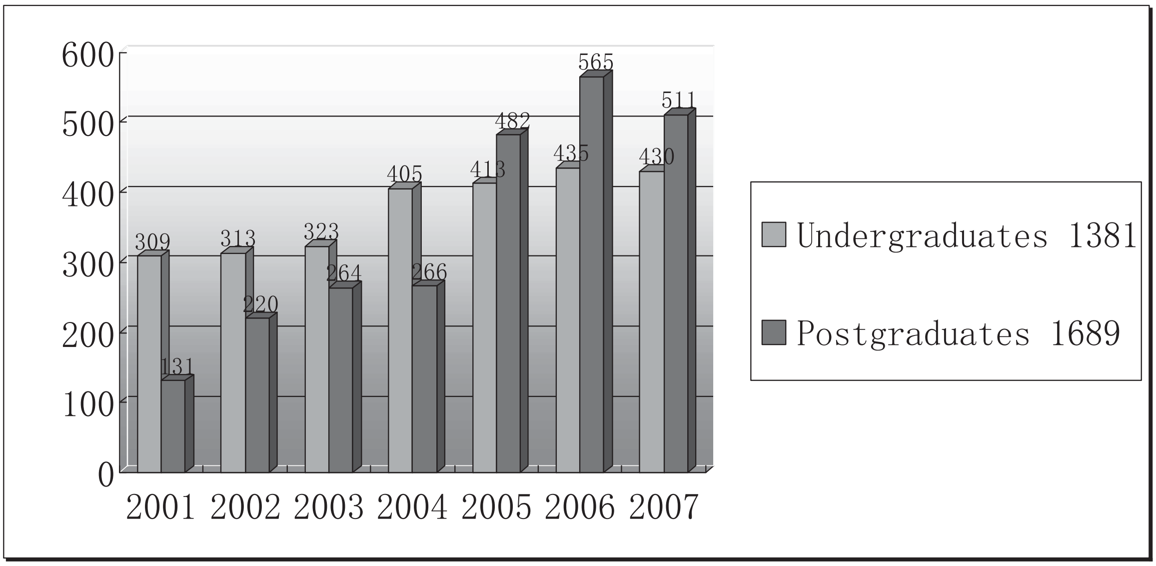
UNIVERSITY OF SCIENCE AND TECHNOLOGY BEIJING

Faculty in School of Materials Science & Engineering

Professors	78
Associate professors	65
Lecturers or assistant lecturers	30
Total	173

• Academicians of Academy of Science	3
• Academicians of Academy of Engineering	2
• Changjiang Scholar Program Professors	6
• National foundation for Outstanding Young Scientists	4

Student Enrollments in School of Materials Science and Engineering



Research Themes

Department of Materials Science

- **Optimization and Design of High Temperature Alloys**
- **Simulation and Theoretical Models of Microstructure**
- **Fundamentals and Anisotropy of Materials**
- **Magnetic Materials and Application**

Research Themes

Department of Materials Processing and Control Engineering

1. Advanced Materials Preparation and Processing
2. Materials Formation Processing Control and Simulation
3. Materials Processing Theory and Structure Control
4. New Technology for Materials Processing
5. Metal Solidification and Control Welding
6. Technology of Advanced Materials
7. Mechanism and Control of Crystal Growth

Research Themes

Department of Materials Physics and Chemistry

1. Control of interface property of nano magnetic materials
2. Crystalline defects and new generation structural materials
3. Nano technology and materials
4. Functional Polymer Materials

Research Themes

Institute of Powder Metallurgy

1. Advanced ceramic materials and technique
2. Inorganic nonmetallic functional materials
3. Inorganic nonmetallic structural materials

Research Themes

Center of Corrosion and Protection

1. Environment Induced Fracture
2. System Engineering of Corrosion Control
3. High Temperature Corrosion and Surface Technology
4. Electrochemical Materials and Engineering
5. Assessment and Control of Environmental Fracture

Research Themes

Department of Inorganic Nonmetallic Materials

1. High-Tech Thin Film Materials
2. High Performance Rare-earth Magnetic Materials
3. Bio-functional Materials

Research Themes

Institute of Functional Materials

1. High-Tech Thin Film Materials

2. High Performance Rare-earth Magnetic Materials

3. Bio-functional Materials

2. History of material database in China

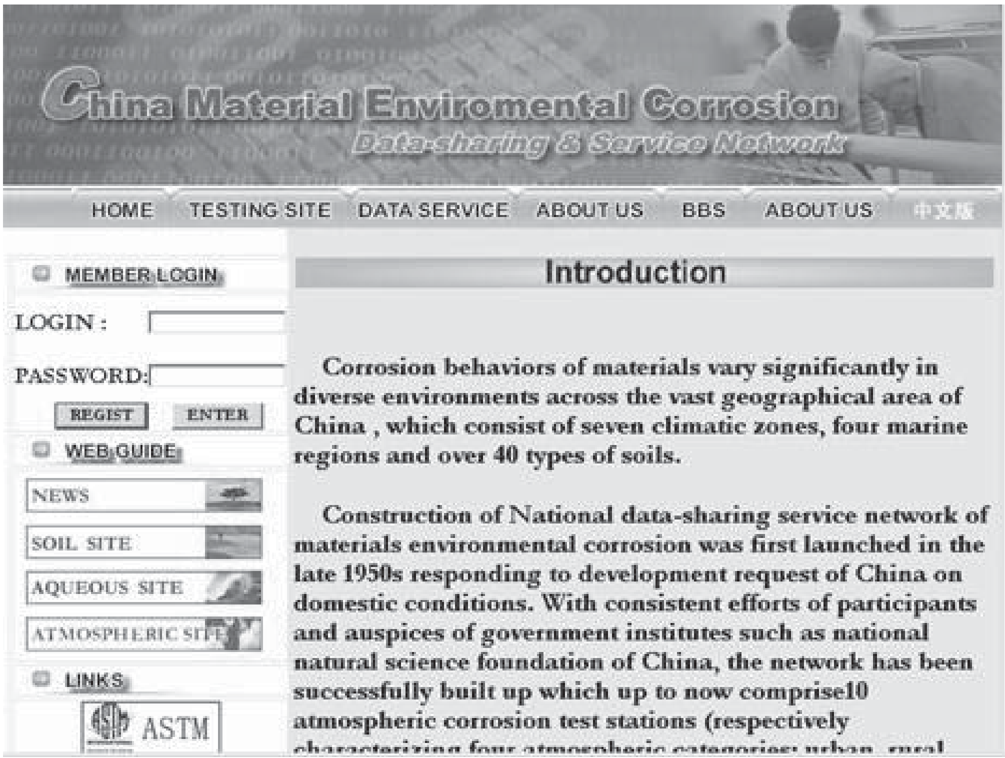
- Construction of Chemical database started in 1979, including more than 10 master databases, in which materials database is one of key components.
- Research on materials database technologies has been carried out since 1980'.
- The first National Materials Database Conference was held in Oct. 1986 in Beijing. Materials database team was founded under the supervision of committee of CODATA China.

MITS 2008 International Symposium on Materials Database

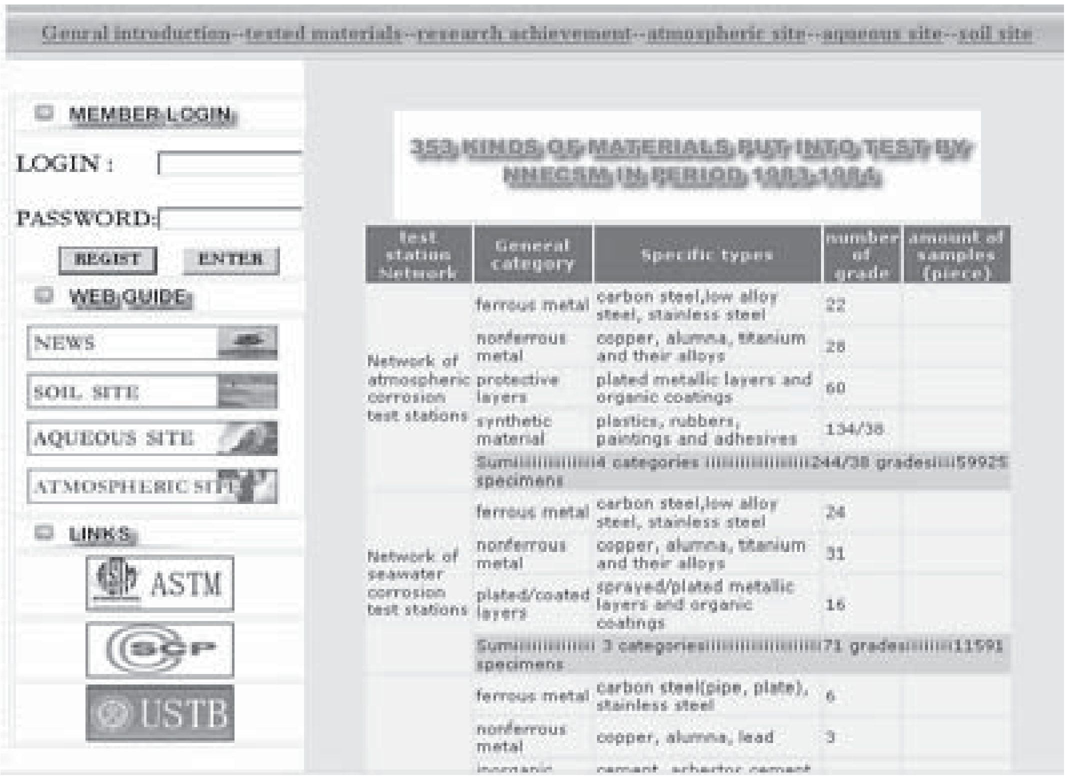
3. Current resources of material databases in China

UNIVERSITY OF SCIENCE AND TECHNOLOGY BEIJING

3.Material Environmental Corrosion Data-sharing & Service Network



Material Environmental Corrosion Data-sharing & Service Network--tested materials

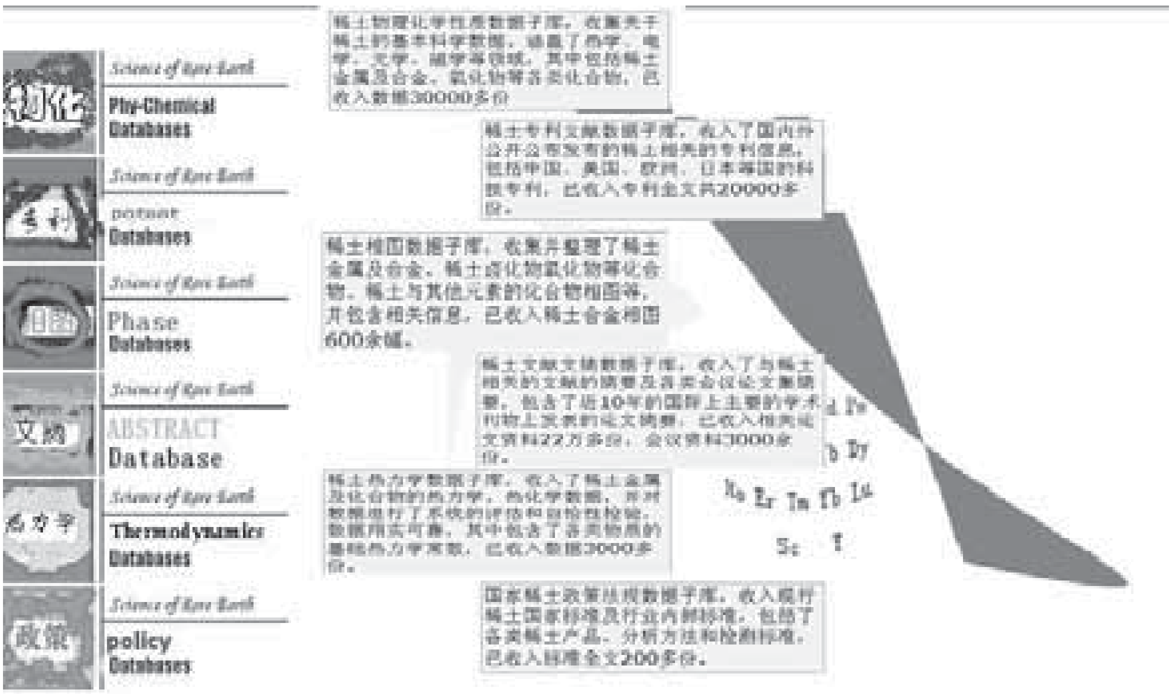


test station Network	General category	Specific types	number of grade	amount of samples (piece)
Network of atmospheric corrosion test stations	ferrous metal	carbon steel,low alloy steel, stainless steel	22	
	nonferrous metal	copper, alumna, titanium and their alloys	28	
	protective layers	plated metallic layers and organic coatings	60	
	synthetic material	plastics, rubbers, paintings and adhesives	134/38	
	Sum!!!!!!!!!!!!!!!4 categories !!!!!!!!!!!!!!!!!244/38 grades!!!!!59925 specimens			
Network of seawater corrosion test stations	ferrous metal	carbon steel,low alloy steel, stainless steel	24	
	nonferrous metal	copper, alumna, titanium and their alloys	31	
	plated/coated layers	sprayed/plated metallic layers and organic coatings	16	
	Sum!!!!!!!!!!!!! 3 categories!!!!!!!!!!!!!!!!!!!71 grades!!!!!!!!11591 specimens			
	ferrous metal	carbon steel(pipe, plate), stainless steel	6	
	nonferrous metal	copper, alumna, lead	3	

Material Data Branch in Basic Science Data Center

- Superalloy database
- Ti alloy database
- Material Corrosion database
- Material Welding database
- Nano Material database
- Tube Material database
- Failure Analysis database

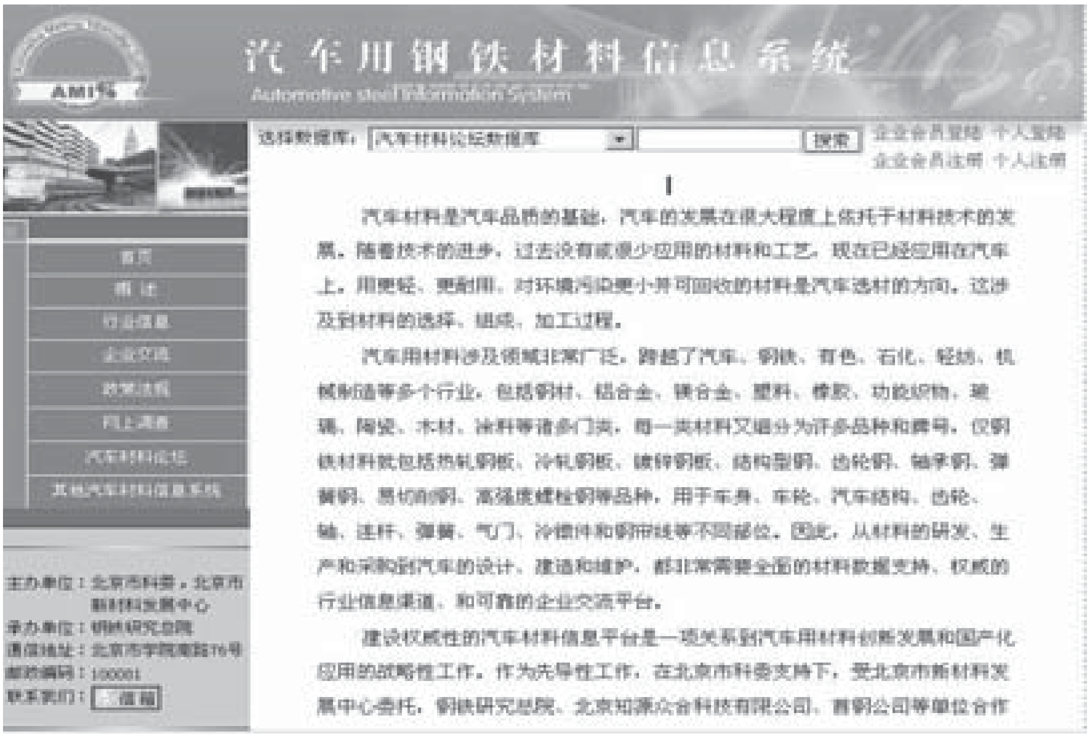
Rare-earth Materials Database



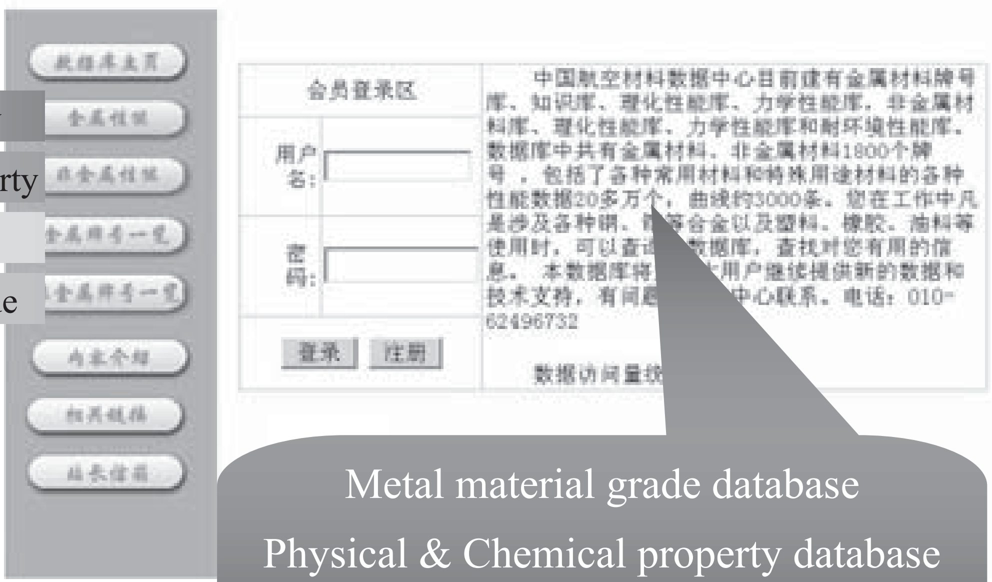
Advanced Manufacturing & Automation Data-sharing Network

Advanced Manufacturing & Automation data-sharing network--search by key word

Automotive Steel Information System



Aeronautical Material data Center



Metal property

Non-Metal property

Metal grade

Non-Metal grade

Metal material grade database

Physical & Chemical property database

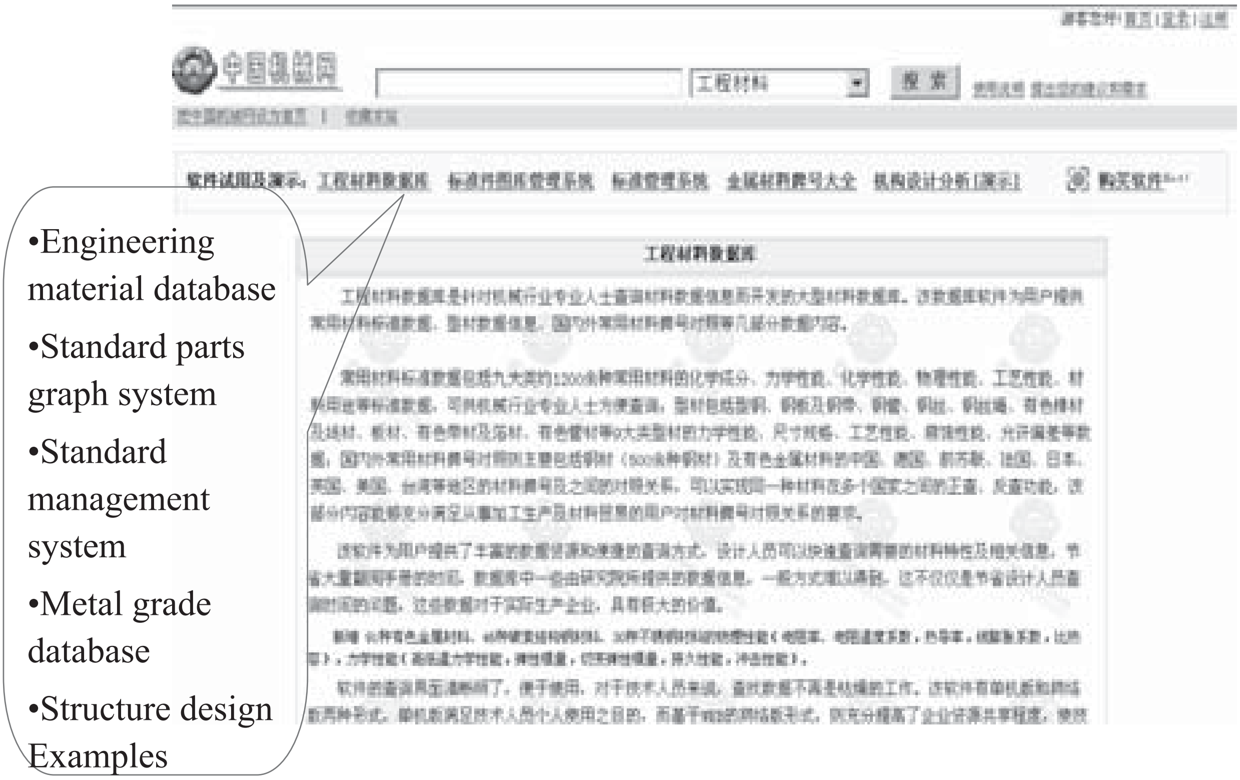
Mechanical property database

Property under environments database

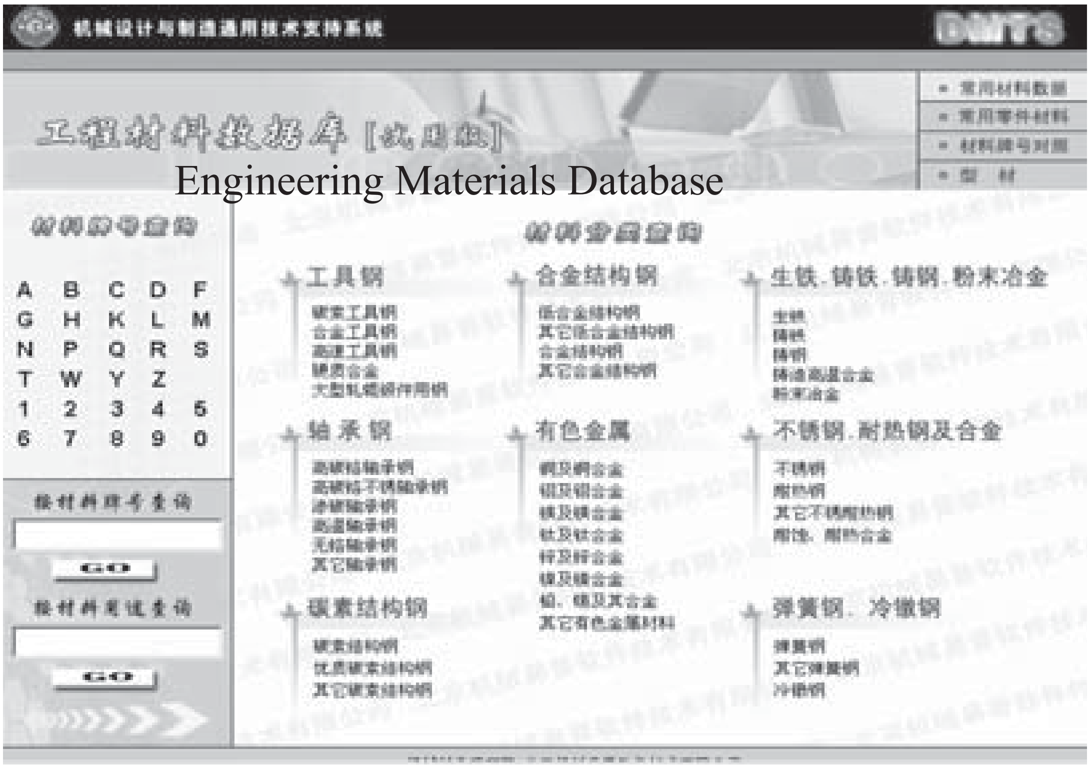
Nanotechnology basic database

- •Patent database
- •Program database
- •Expert database
- •Measurement Technology database
- •Material property database
- •Abstract database
- •Nano device database

China Machinery network



Engineering Materials database under China Machinery Network



Other Material Databases supported by national projects

- New materials database, comprised of 5 sub-databases on new metals and alloys, fine ceramics, polymer materials, advanced composite materials and amorphous materials.
- Superhard materials and abrasive materials database
- Packaging material database
- Alloyed steel Database
- Membrance seperation database

⋮

Nano Material Database under Shanghai R&D Public Service Platform

Wansteel website

Wansteel website--search by grade

Powder Metallurgy Business Information website

Characteristics of Material Databases in China

- In large amount
- Supported by national and local government, and private sectors.
- Dispersed in different branches, areas and institutions
- Not comprehensive and lack of systematicness
- Most are in Chinese, without English version.

4.Strategy and policy of material database in China

- National Guidelines for Medium- and Long-term Plans for Science and Technology Development (2006-2020).
- Promote the integration of scientific data resources generated and accumulated by national research projects, to make them more open and accessible based on the requirements of scientific and technological innovation.

Objectives by 2010 year

- Build a data management and sharing service system with a three-tier structure consisting of 40 scientific data centers or networks, 300 master databases and one portal.

- Cover six major fields: natural resources and environment, agriculture, population and health, basic and frontier sciences, engineering and technology, and regional scientific and technical research.

Objectives by 2020 year

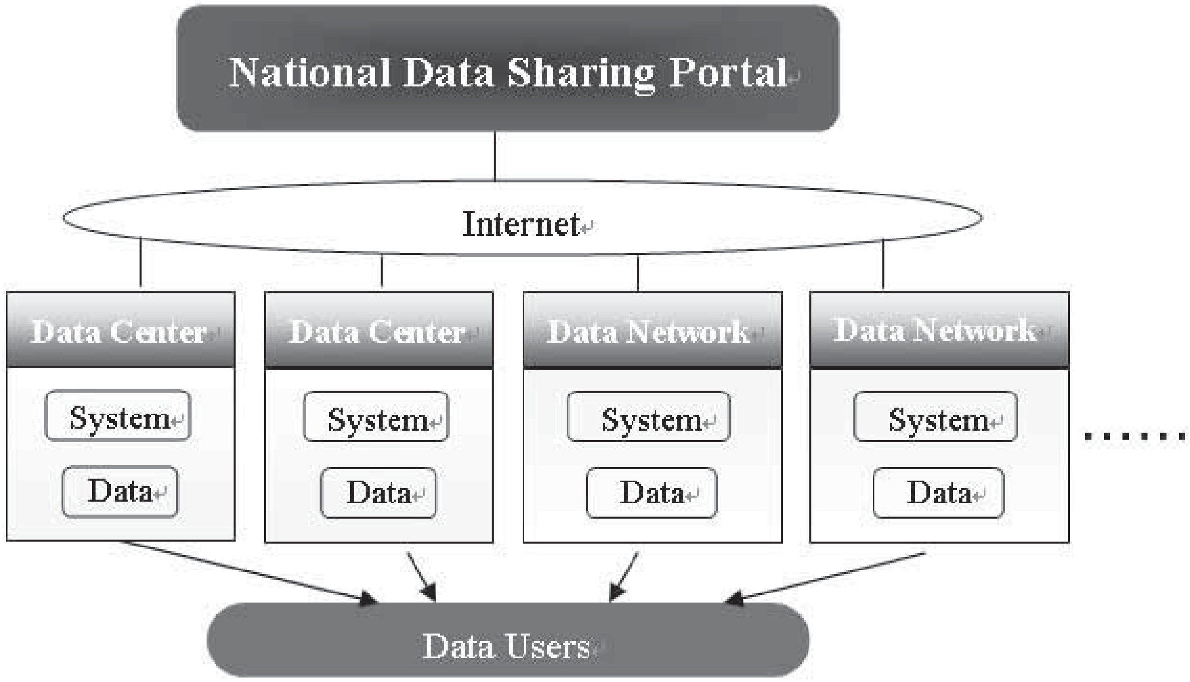
- establish a networked scientific data management mechanism and a data sharing service system.
- establish data policies, regulations and standards, and implement an operational sharing mechanism.

Strategy and policy of material database in China

- National Scientific Data Sharing Program (SDSP) in 2002, as an important part of the science and technology infrastructure platform of China

- Workshop on Strategies for Open Access to and Preservation of Scientific Data was held in Beijing in 2004, with over 100 participants from 12 countries.
- 23 laws, rules and regulations which are instructional, general and special are released at the national level.

National Scientific Data Sharing Program



MITS 2008 International Symposium on Materials Database

5. Introduction to Materials Scientific Data Sharing Project of China

Goal and Vision

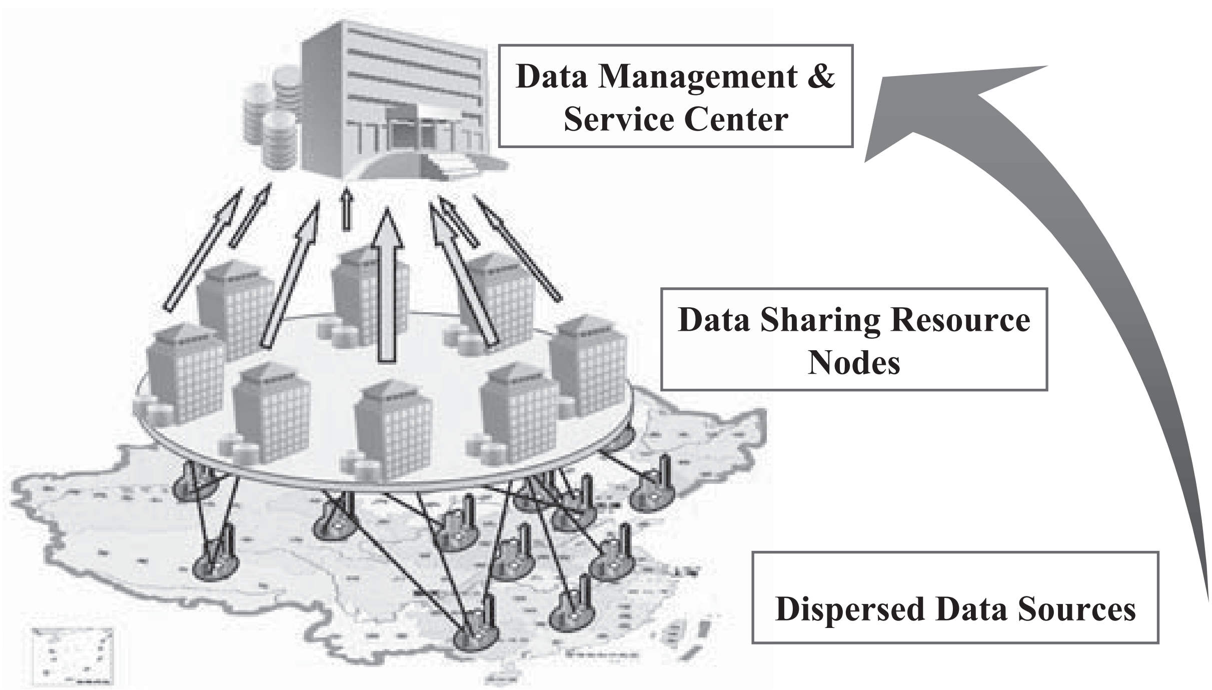
Integration of materials scientific data resources, to make them more open and accessible according to the requirements of scientific and technological innovation.

Establish materials data sharing network

- A series of data sharing resource nodes
- Center of material data management and Service
- Standards and specifications for material data sharing

Provide data sharing and intelligent services for different users, including data navigation, download, intellectual search, data mining, etc.

National Materials Scientific Data Sharing Project



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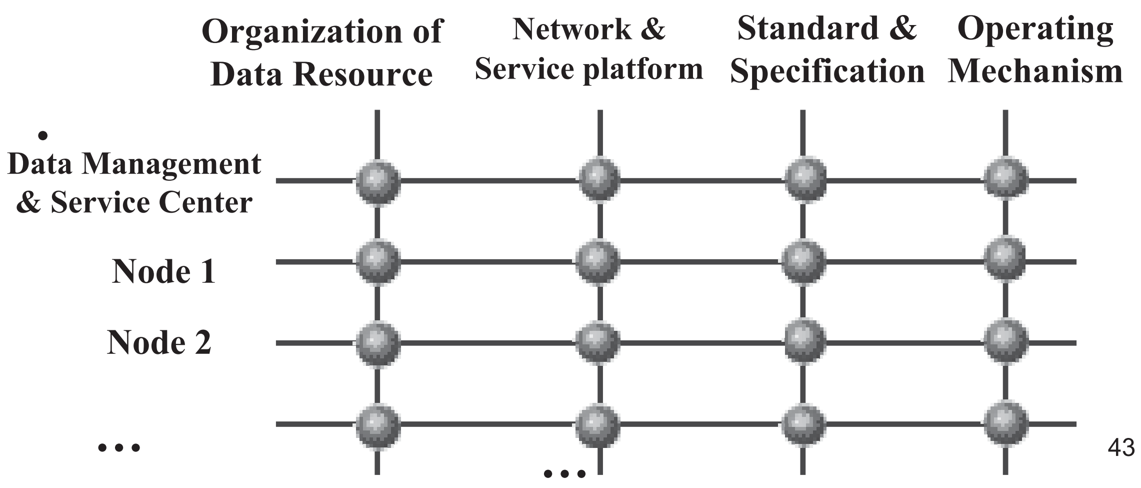
Contents of Construction

- Data Management & Service Center
- 8 Data Sharing Resource Nodes

← Data resource / Network & service platform / Standards & specifications / Operating mechanism



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Portal of Materials data sharing network

- **Data Services**: Data Query; Keyword Query; Material Selection; Materials Brand Query; Performance Prediction
- **User Management**: Metadata Query; Heterogeneous Data; Failure Analysis
- **Data Collection**: Specification; Data submitting; Metadata Browsing; …; …
- **Sharing Movement**
- **Materials Forum**: News; Notice and Post; Academic Frontiers; Market Information; …
- **Standard Specification**: Database Standard; Metadata Standard; Data Element Standard; Data Junction Standard; …
- **Literature**: Construction Specification Of data Sharing Network
- **Auxiliary Tools**: Unit conversion; Terms Index; Brand Standard; Hardness Conversion; Periodic Table of Elements; …

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Portal of Materials data sharing network

- Search by catalog / keywords
- Data query / metadata query
- Intelligent service

- By properties
- By materials brand name
- By chemical composition
- By materials application
- Advanced query (by all above)

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Data services---Data query

Query by properties

- •Mechanical property
- •Physical property
- •Heat treatment
- •Multi properties

Data services---Data query

Query by mechanical property

specify mechanical property ranges

Data services---Data query

Query by heat treatment type

select feature points and curves which will be shown in the query result

Data services---Data query

Example of query by material compositions

Input the percentage range of elements

Query Result in chat view

Query Result in table view

Data services---Data query

Advanced query

User can make query in a very convenient way, and able to input conditions on multi dimensions of materials.

Material type

Application

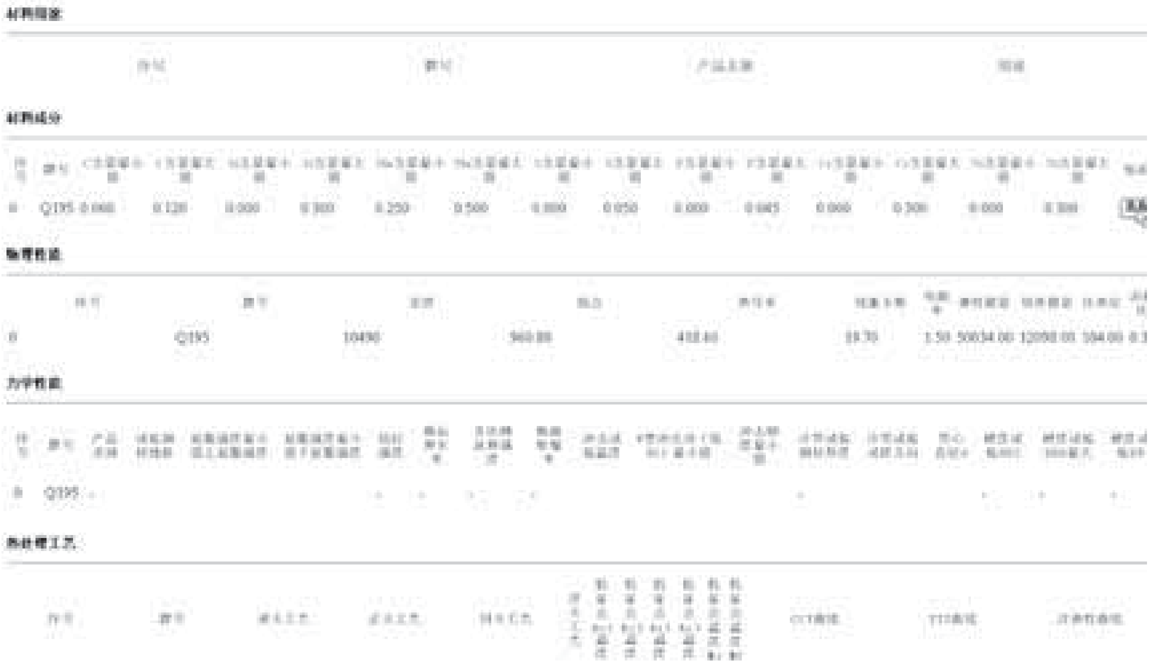
Mechanical property

Physical property

Composition

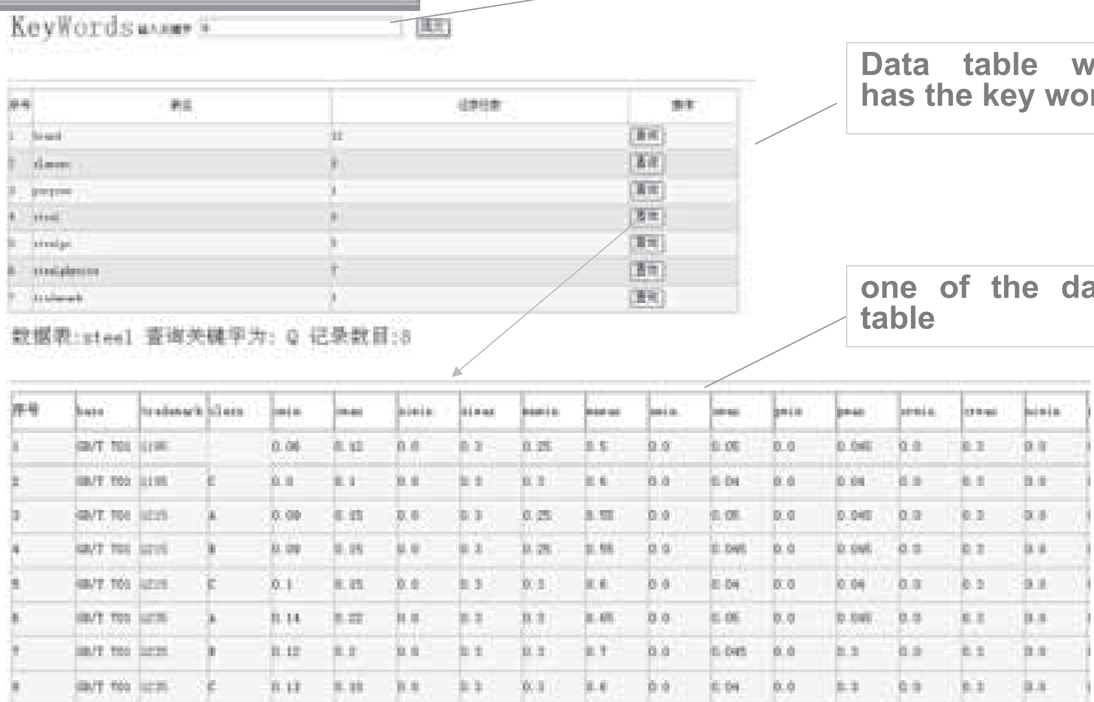
Data services---Data query

Example of query result



Data services---Data query

Query by key words



Input key words

Data table which has the key words

one of the data table

Data services---Metadata management

Metadata management

- Submit metadata
- Upload dataset
- Search metadata

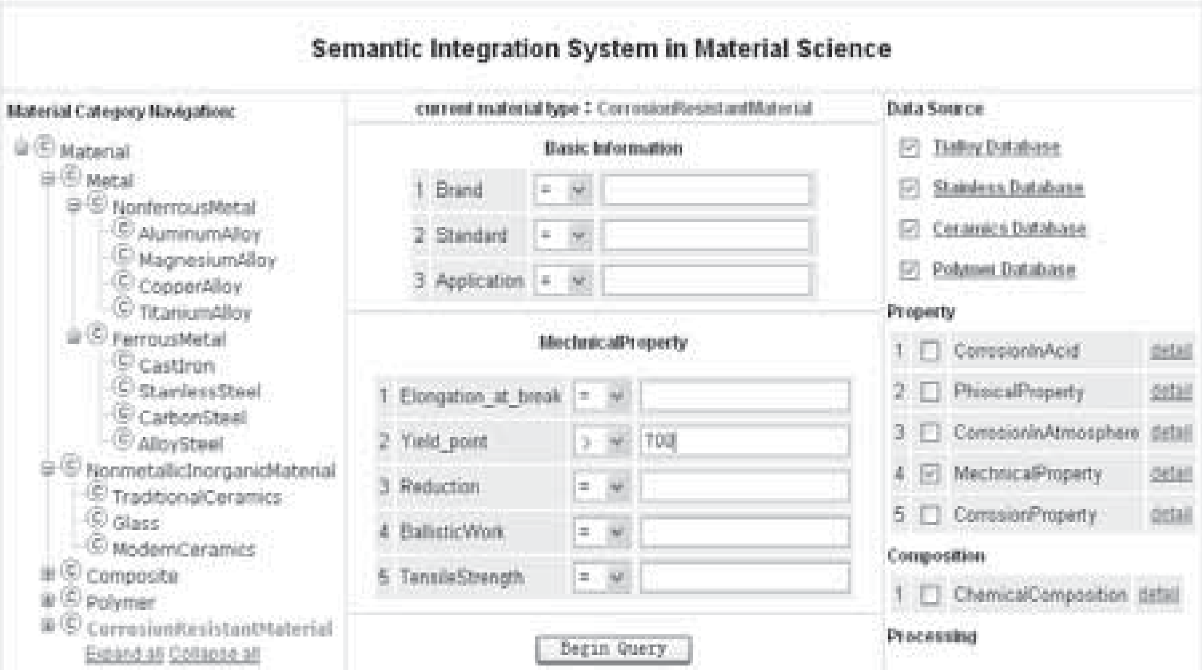
Search metadata

Specification

Materials database design specification

- **Terms and abbreviation**
  - **Domain vocabularies**
- **Naming rules for materials data object**
  - **Table, column, index, view, trigger...**
- **Design flow for materials database**
  - **Conceptual design, logical design, physical design**
- **Practical Guidance for domain users**
  - **Design principles, maintenance, security, documents…**
- **Design Example**

Key problem---
Query over heterogeneous data sources



Concept hierarchy

①select materials type

Conditions

input query conditions

Properties

select related properties

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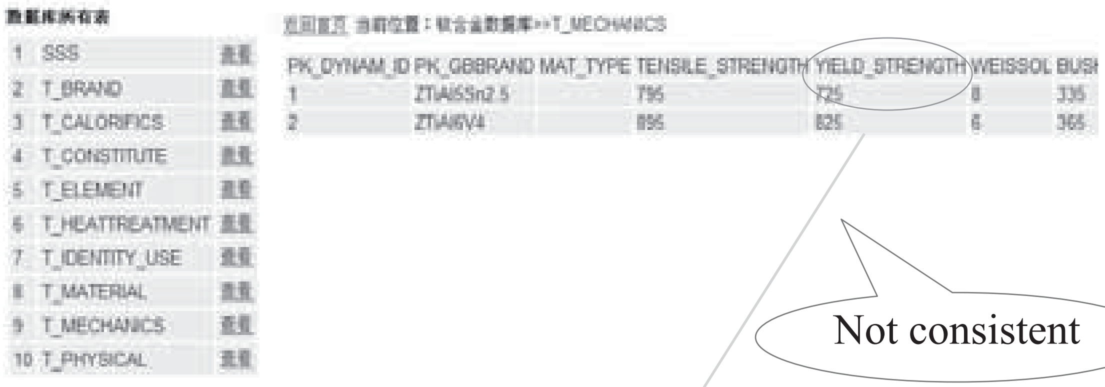
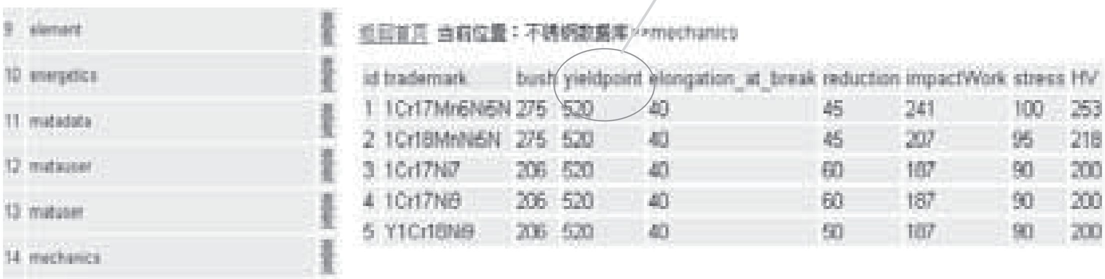
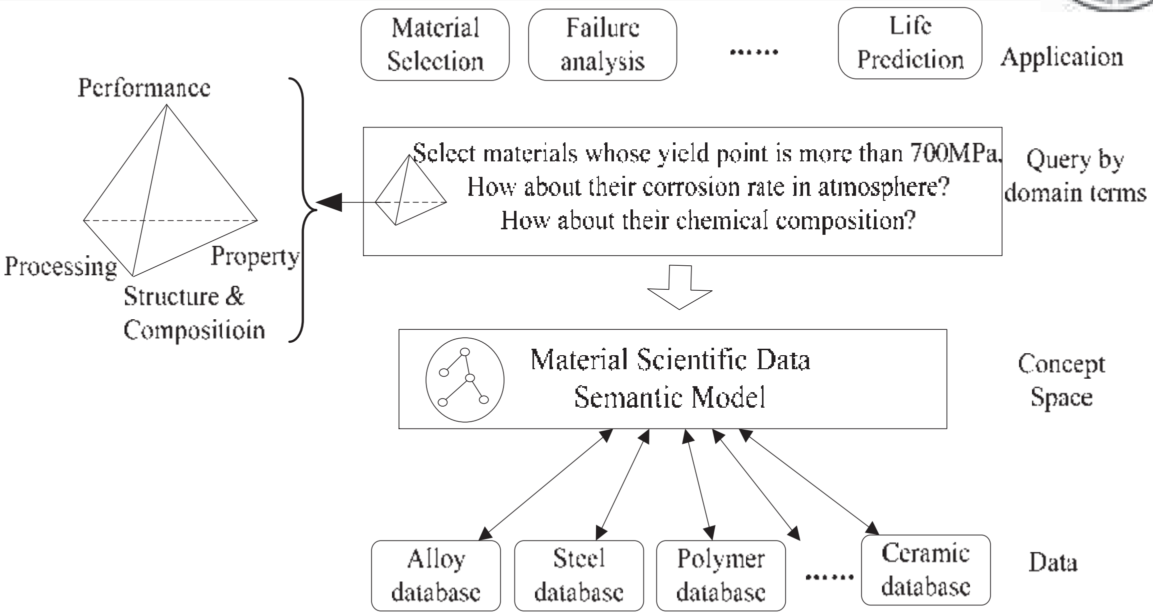
Query system over heterogeneous data sources



Not consistent



Solution to Query system over heterogeneous data sources



Semantic model and integration method are testified effective for integrating scientific data in materials science.

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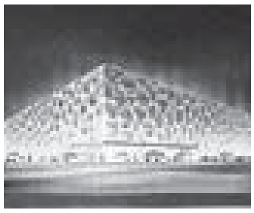
6. Summary

- National material scientific data sharing network play an important role to leverage the abundant resource of materials data, to meet the requirement of scientific and technological innovation in China.
- National material scientific data sharing network is under construction, with the emphasis on integration of dispersed data resources, establishment of relevant standards and specifications, data evaluation and effective long-term operations, to make them available to the general public.
- We would like to share our experience with others to promote international communication in Asia and worldwide.

UNIVERSITY OF SCIENCE AND TECHNOLOGY BEIJING

Welcome to 2008 Olympic Games Beijing

•3 km



The gym for judo of 2008 Olympic Games is built on the campus of USTB.

Indian Materials Database for Scientists, Engineers and Industries

R. K Dayal, S. Rajeswari, R.V. Subba Rao, A. Sambasiva Rao, S. A. V. Satya Murty and Baldev Raj

Indira Gandhi Centre for Atomic Research
Kalpakkam -603 102 (India)

Corresponding author's email address: rkd@igcar.gov.in

A project consisting of development of Indian Materials Database for Scientists, Engineers & Industries through compilation of materials property data available in different laboratories situated in India has been taken up. The importance of the common database was realized as large source of data on creep, fatigue, tensile, fracture and corrosion properties on different structural materials have been generated in Indian Laboratories during past four decades. Indian laboratories are now self sufficient to provide vital data needed for power, space and chemical industries. There is also a large scope for Indian industries to use this database. Availability of materials database is of high relevance as huge investment in energy, chemical and other sectors and new materials are being explored. Uniqueness of this database is its authenticity, since these are already published data. The main emphasis of the work is the compilation of the data from different laboratories, linking the laboratories for periodic updating of the data and access of the data to the scientists and engineers. The database centre has a scope of extending to other materials properties. Indira Gandhi Centre for Atomic Research (IGCAR) Kalpakkam, which has carved a special name for itself in the international community of metallurgists due to its contributions in the area of materials science, the Indian Institute of Metals (IIM), a professional body on metallurgical activities and the Indian National Science Academy (INSA), a professional body for scientific activities in India have been identified as the nucleators of this effort of setting up of a centralized materials database catering to materials and properties to start with. In the next 5-10 years, number of databases for this centre is expected to grow to about 500 and the volume of database may grow to a few terabytes.

With typical sets of data on mechanical and corrosion received from different institutes, one web-based portal has been attempted and successfully implemented. With the help of respective experts, the presentation methodology on the web is decided based on the types of data. The site prepared this way has provision to accept data that is authentic and relevant through proper identification of the sender as well as the data. To achieve this, registration of users is made mandatory and minimal data necessary are collected. The site would additionally have details about the journals where these data were published, bio-data of the authors and links to relevant sites etc. In this paper the salient design features of the database, methodology, and utilization along with a demonstration of web-based portal are presented.

Indian Materials Database for Scientists, Engineers and Industries

R.K. Dayal
Indira Gandhi Centre for Atomic Research
Kalpakkam (India)

Importance of Indian Materials Database

- **Large source of Data on Creep, Fatigue, Tensile, Fracture and corrosion properties on different structural materials have been generated in Indian Laboratories**
- **Indian laboratories are self sufficient to provide vital data needed for power, space and chemical industries**
  - **Large source of scientific data available in many fields should be easily accessible for the use of other scientists for their benefit and to avoid duplication of data generation**
  - **Scientist and engineers should have a knowledge of frequent updating of the data generated by national laboratories**
  - **Motivation of Scientists on availability/utilization of their data (*increase of impact value of the data*)**
  - **A large scope for industries to use this database**

Importance of Indian Materials Database

- **Collaborations through long-distance and improvement in the quality & reliability of data**
- **Building and verifying theoretical models and development of new materials**

- *In India, the availability of materials database is of high relevance as huge investment in energy, chemical and other sectors and new materials are being explored*
- *The efforts on the formation of Indian database are to be in parallel and in synergy with rest of the world for our own industrial growth*

Database Features:

Data quality
generation of basic data based on recognized/ standard test methods

Data accessibility
information of data and source of data/ laboratories/ equipment/ specialisation

Data archiving
Collection of old classic materials data

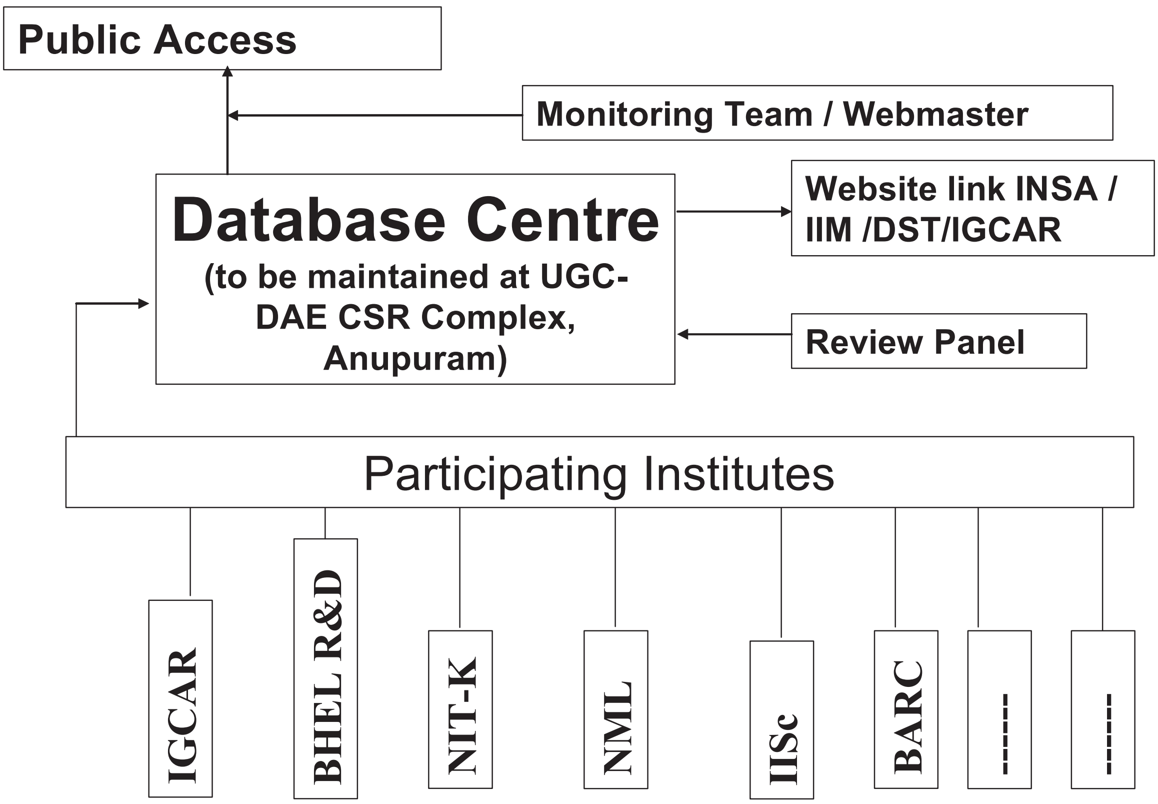
Plant experience; failure analysis

Industries materials product specifications information

Comparison of developed Indian Database on Materials with other databases

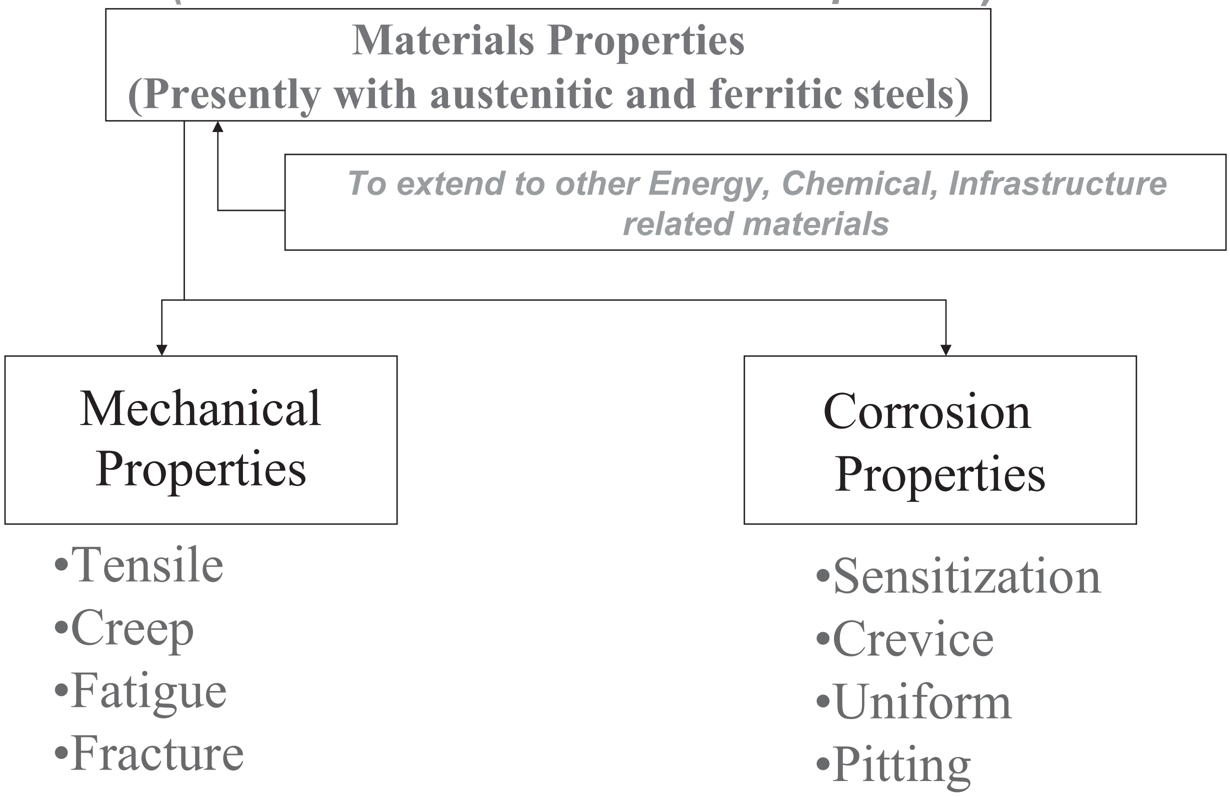
- **Most of the databases world wide give materials datasheets in form of PDF files from laboratory and industrial catalogue**
- **Features of searching such as properties with respect to material, environment conditions etc are not available in most of the databases**
- **Indian database is developed with interlinking of different national laboratories**
- **Database prepared on properties stored in individual field structure from which a desired report can be built depending on the search parameters**

Structure of Indian Database On Materials Properties

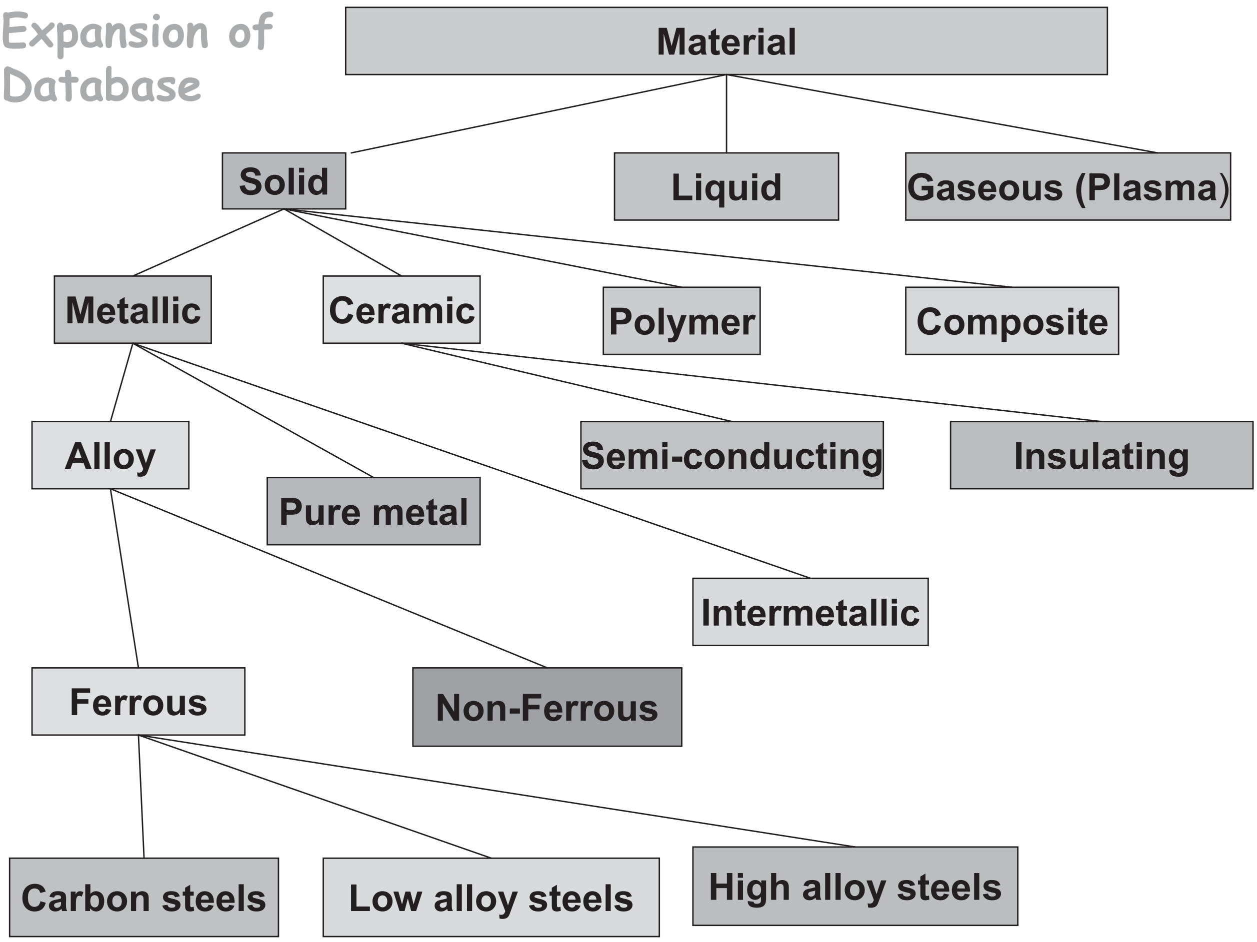


Indian Materials Database (IMDB)

(Mechanical and Corrosion Properties)



Expansion of Database



Project proposal to Department of Science and Technology, Government of India

Project Title: Setting up of an Indian Materials Database for Scientists, Engineers and Industries

- **This database would be available to scientific community all over the world**
- **This data store would be the first of its kind in India where all Materials Data in India would be available at one place**
- **Uniqueness of this data would be its authenticity, since these are already published data.**

Leading Institutes managing the database

Indira Gandhi Centre for Atomic Research (IGCAR)

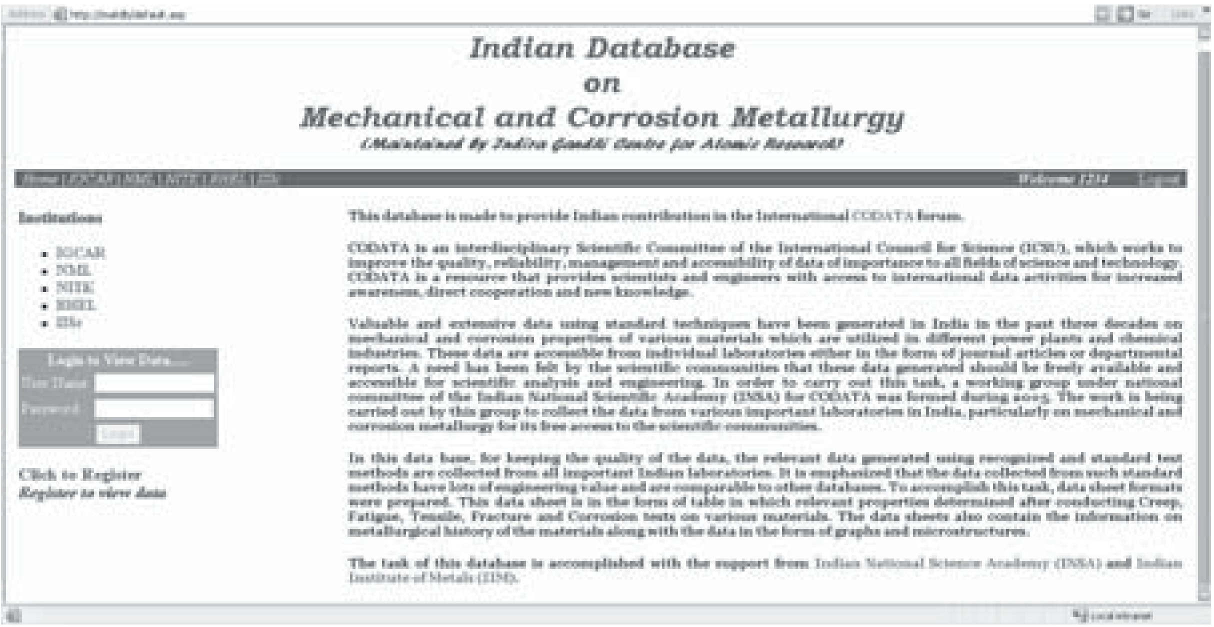
valuable mechanical and corrosion property data on various structural materials like austenitic stainless steels and ferritic steels have been generated which have been used to design components for nuclear plants

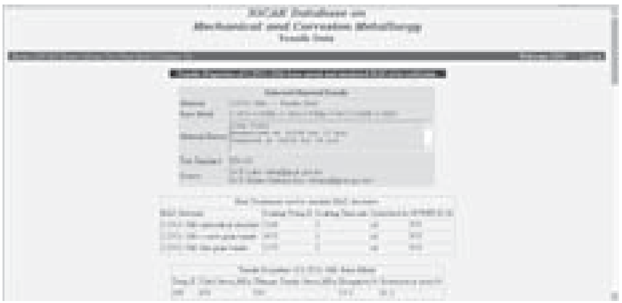
Indian Institute of Metals (IIM)

A professional body for metallurgists in India. It has recently crossed the milestone of 60 years of its glorious existence more than 12000 members

Indian National Science Academy (INSA)

promotes public awareness and understanding of science Acting as links between the scientific community and the planners, they advise the governments on critical issues





Direction in the development of Indian Database

- **Coordinators from different zones:**

•South:	IGCAR,Kalpakkam
	NIT-K
•East:	NML, Jamshedpur)
	IIT-Kgp
•West:	BARC,Mumbai
	IIT-B
•North:	IIT-R
	IIT-K
•Central	BHEL R&D
	VNIT Nagpur

The database is expected to grow

Participation from

More institutes

Industries (product specs display)

Additions on Chemical and Physical properties

In next 5-10 years

Number of databases may grow to 500

Volume of data base may grow to a few terabytes

Maintenance of the centralised Database centre (IMDB) with full time staff

Thanks

Data-Driven Materials Design using Pauling File Binaries Edition

P. Villars[1*] and S. Iwata[2]

[1] Material Phases Data System (MPDS), CH-6354 Vitznau, Switzerland
[2] The University of Tokyo, Tokyo, Japan
[*] Corresponding author's e-mail address: villars.mpds@bluewin.ch

Abstract
We postulate *"Structure-sensitive material properties are quantitatively described practically by the elemental-property parameters atomic number AN and 'periodic number' PN (or simple mathematical functions of them) of the constituent chemical elements"*. This generalization is an important step to strategically explore structure-sensitive materials properties of strongly correlated large scale complex systems, linked together with large materials databases such as the Pauling File Binaries Edition [1].

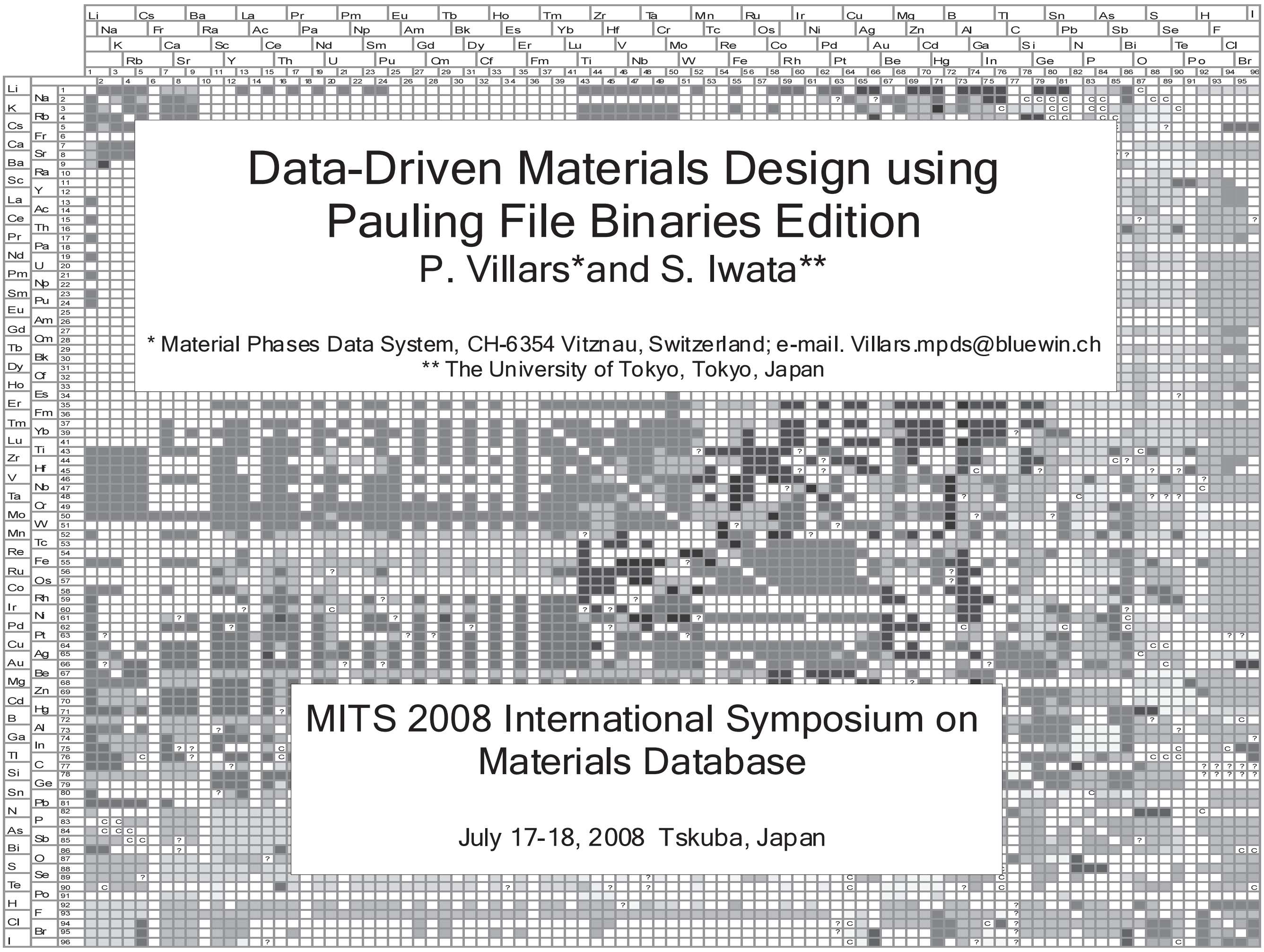
The PN represents a different enumeration of the chemical elements, emphasizing the role of the valence electrons. In contrast to the AN, PN depends in details on the underlying Periodic Table of the chemical elements. As a first result we describe the elemental-property parameters 'atomic size SZ_a' and 'atomic reactivity RE_a', derived from fits to various experimental and theoretical data sets. These two parameters can be approximated as simple functions of AN and PN:

$$SZ_a = k_{SZ}\,[\log(AN+1)][k_{PN} - (\log PN)^3] \quad (1)$$
$$RE_a = k_{RE}\,\{[\log(AN+1)][k_{PN} - (\log PN)^3]\}^{-1} = k_{SZ}\,k_{RE}\,(SZ_a)^{-1} \quad (2),$$

where k_{PN} is a scaling factor, and k_{SZ}, k_{RE} are fit parameters for a fit to experimental data. We argue that all elemental-property parameters are derived from AN and PN. On the example of compound formers/nonformers in binary to quaternary chemical systems we demonstrate that a quantitative link exists between the material property 'formers/nonformers' and AN, PN (or simple functions of both) of its constituent chemical elements. With a second example the atomic environment types AETs (coordination polyhedra) realized in binary to quaternary inorganic compounds we confirmed above made statement. The PN was successfully used to classify the AETs in a generalized ($PN_{(central\ atom)}$ versus $PN_{(coordinating\ atoms)}$) – AET matrix sub-dividing the [central atom–coordinating atoms] combinations where different atomic environment types occur into distinct AET stability domains. The impossible [central atom-coordinating atom] combinations are identical to those where no compounds are formed in equi-atomic binary systems.
Encouraged by the success shown above we propose to bring together different theoretical models (first principles calculation, CALPHAD, data mining, discovery approaches), and the Pauling File Binaries Edition (experimental facts). This with the aim to create a platform, which will allow an interaction between models and experimental data taking into account elemental-property parameters of its constituent chemical elements. Such a platform will become a useful tool to design materials with pre-defined application properties.
To achieve our objectives we will focus on the following points:

- Strategic search for general correlation's using the relatively complete set of experimental data available for binary systems. This with the aim to create a link to the 'sparse' information available for multinaries by developing extension techniques.
- Generation of calculated/derived data, including in particular domains where experimental data are missing.

References
[1] P. Villars, K. Cenzual, F. Hulliger, H. Okamoto, J. Daams, K. Osaki A. Prince and S. Iwata, "Pauling File (LPF), Binaries Edition" CD-ROM, ASM International, Materials Park, OH, 2002



Data-Driven Materials Design using Pauling File Binaries Edition

P. Villars*and S. Iwata**

* Material Phases Data System, CH-6354 Vitznau, Switzerland; e-mail. Villars.mpds@bluewin.ch
** The University of Tokyo, Tokyo, Japan

MITS 2008 International Symposium on Materials Database

July 17-18, 2008 Tskuba, Japan

Distinct Phases Level Materials Databases

Below is given the only Materials Database of that type:

Database Structure: Distinct Phases Level (Distinct Phases per Chemical System)

Link between the 4 fundamental materials data: Structure, Diffraction, Physical Property and Constitution; Data are fully linked through distinct phases

Advantages: Data linked and under the same computer environment enabling to search for cross relations between these data

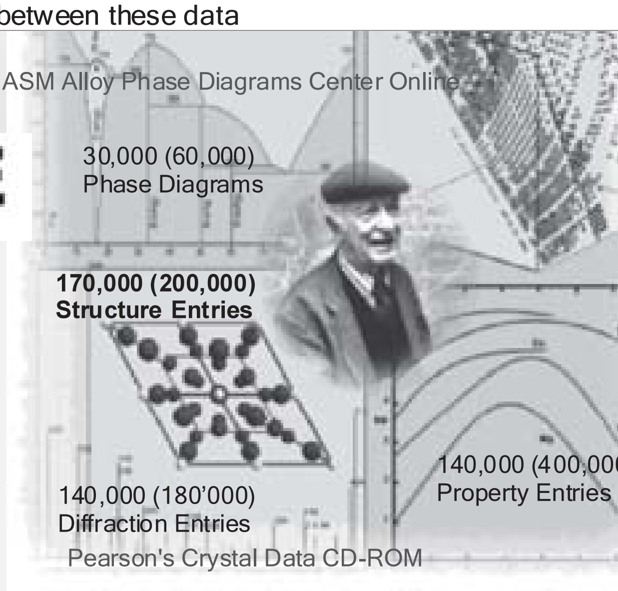
PAULING FILE
Inorganic Materials Database and Design System

Binaries to multinaries

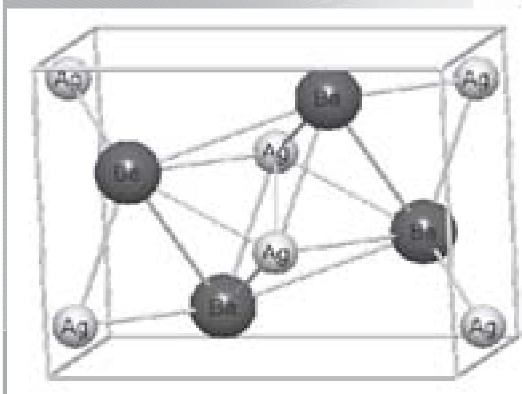
Non-metals, metals, intermetallics, ceramics, inorganics

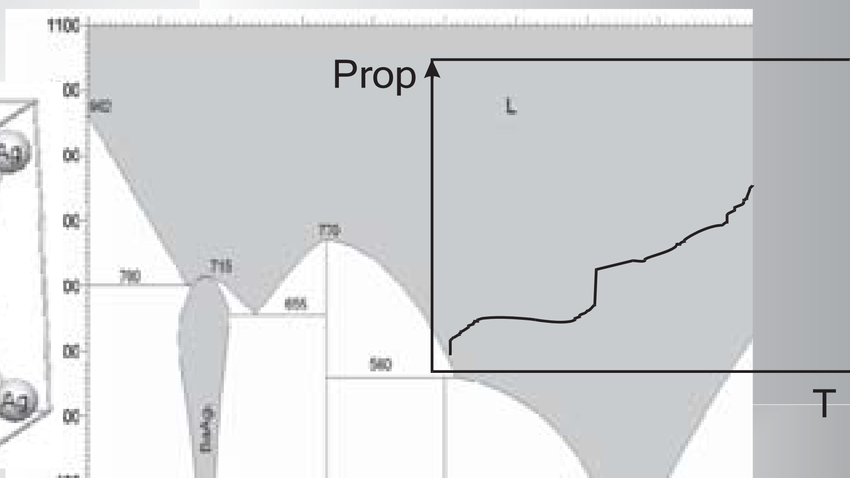
Edited by:
P. Villars (editor-in-chief)
K. Cenzual, J. Daams, F. Hulliger, T. Massalski, H. Okamoto, K. Osaki, A. Prince† (section-editors)
S. Iwata (project coordinator)

PAULING FILE Binaries Edition CD-ROM



'Fundamental Materials Data' Statistics (LPF + L&B)

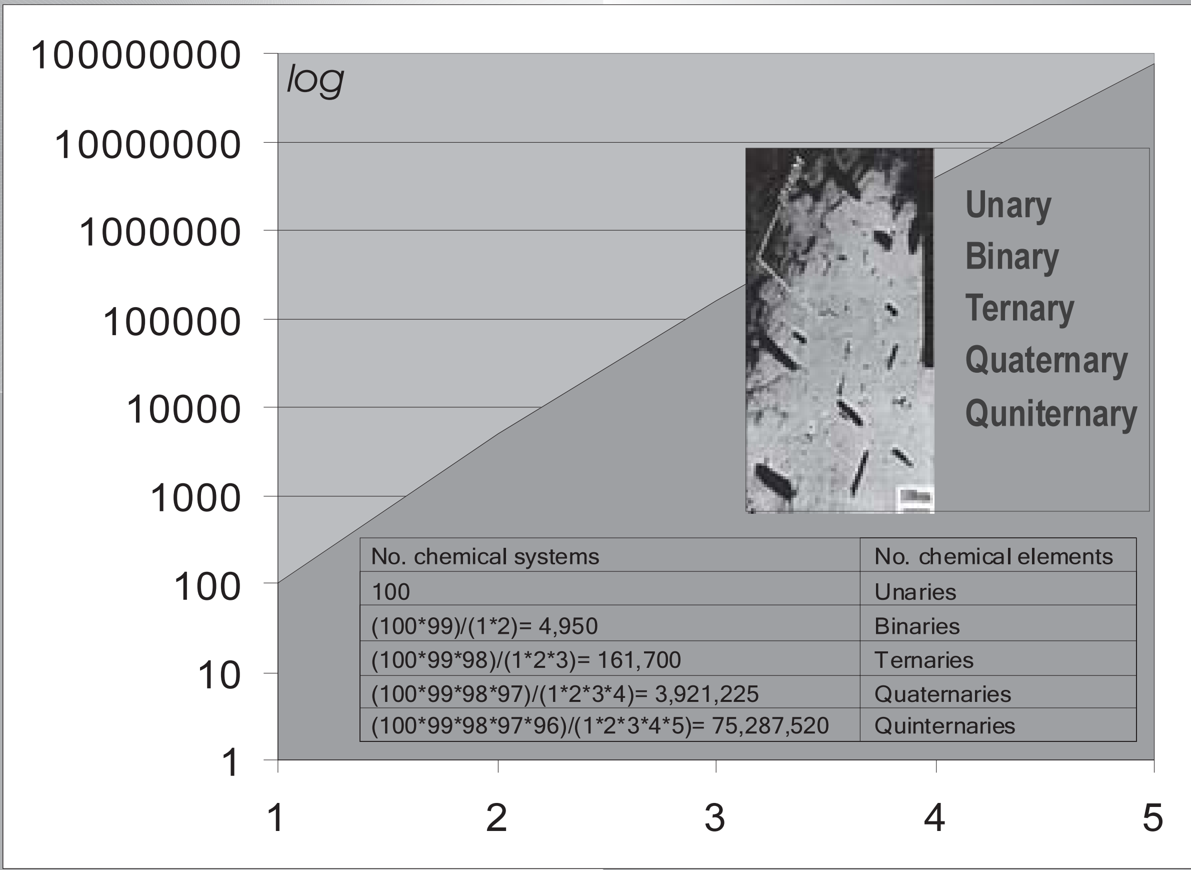




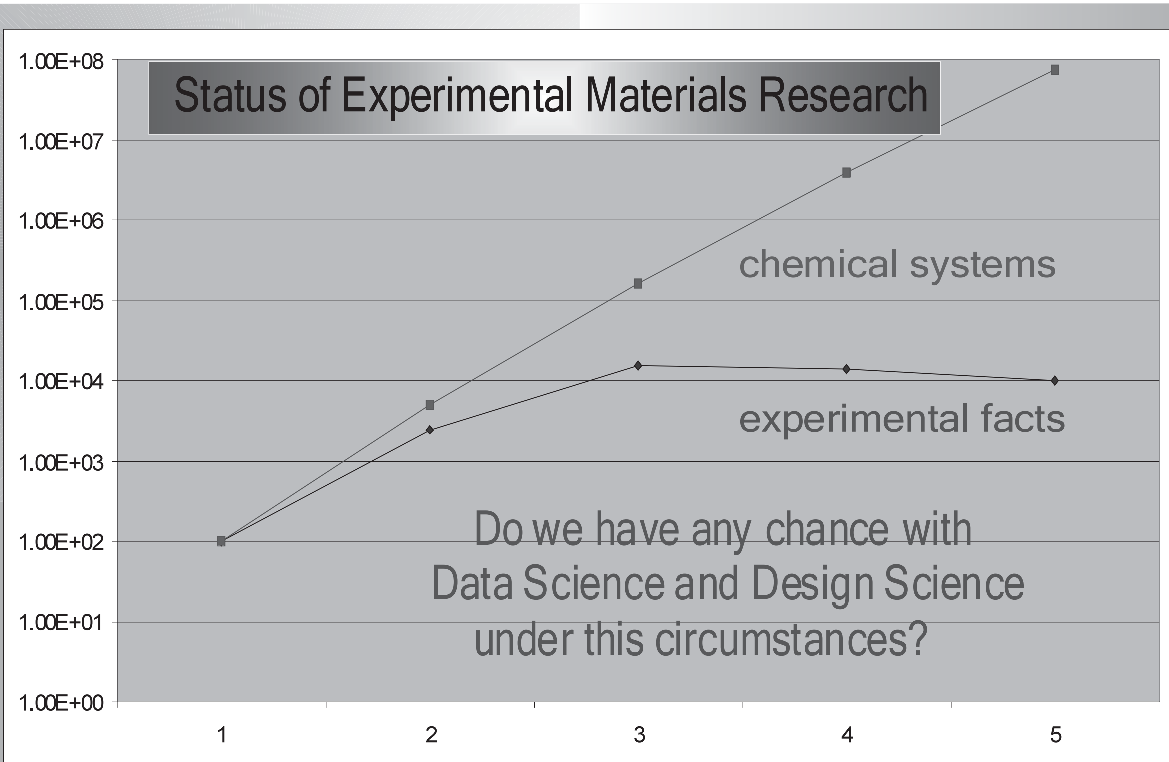
No. of chemical elements	structure / diffraction	property data sets	constitution data sets
Unaries	94	101 (LPF) / 101 (L&B)	94
Binaries	12,506	11,181 (LPF) / 12,000 (L&B)	2,324
Ternaries	35,027	12,972 (LPF) / 25,000 (L&B)	4,082
Quaternaries	26,526	6,009 (LPF) / 7,500 (L&B)	4,000
Quinternaries	21,330	2,953 (LPF) / 7,500 (L&B)	4,000
Sixternaries	4,000	1,000 (LPF) / 2,000 (L&B)	1,000

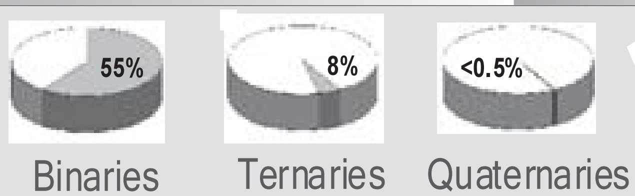
World largest databases covering world literature

No. chemical systems vs. No. chemical elements

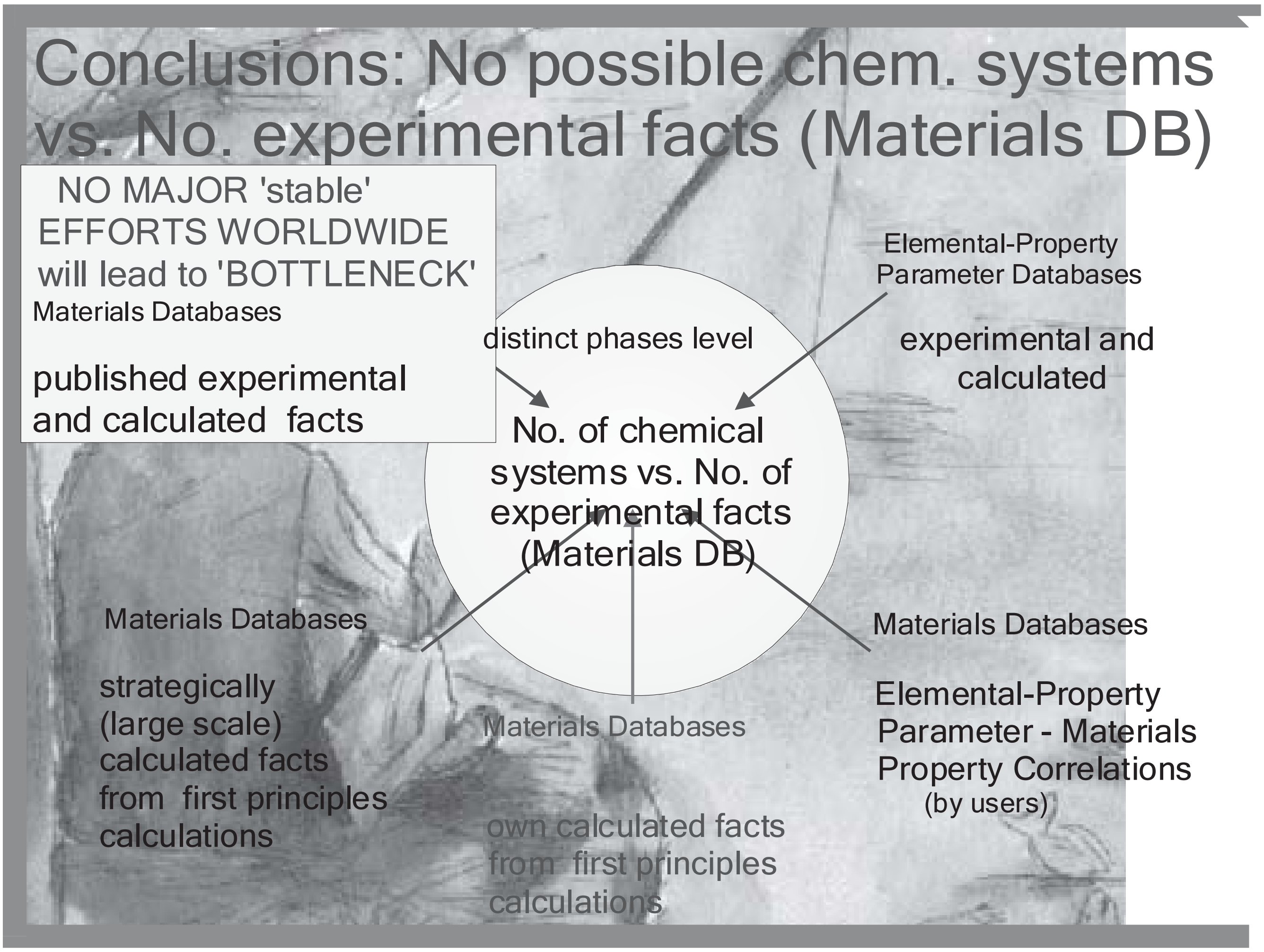


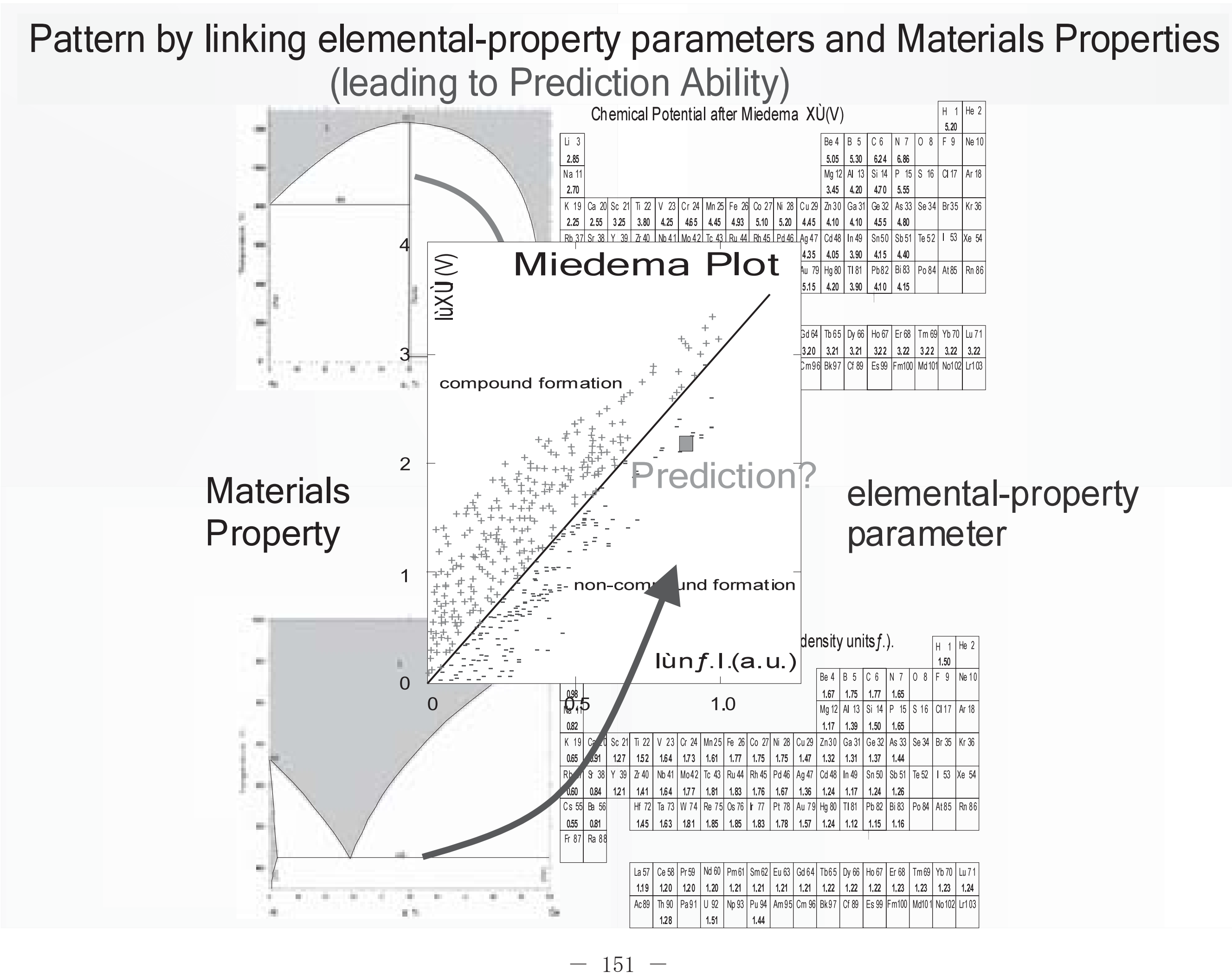
No. chemical systems	No. chemical elements
100	Unaries
(100*99)/(1*2)= 4,950	Binaries
(100*99*98)/(1*2*3)= 161,700	Ternaries
(100*99*98*97)/(1*2*3*4)= 3,921,225	Quaternaries
(100*99*98*97*96)/(1*2*3*4*5)= 75,287,520	Quinternaries

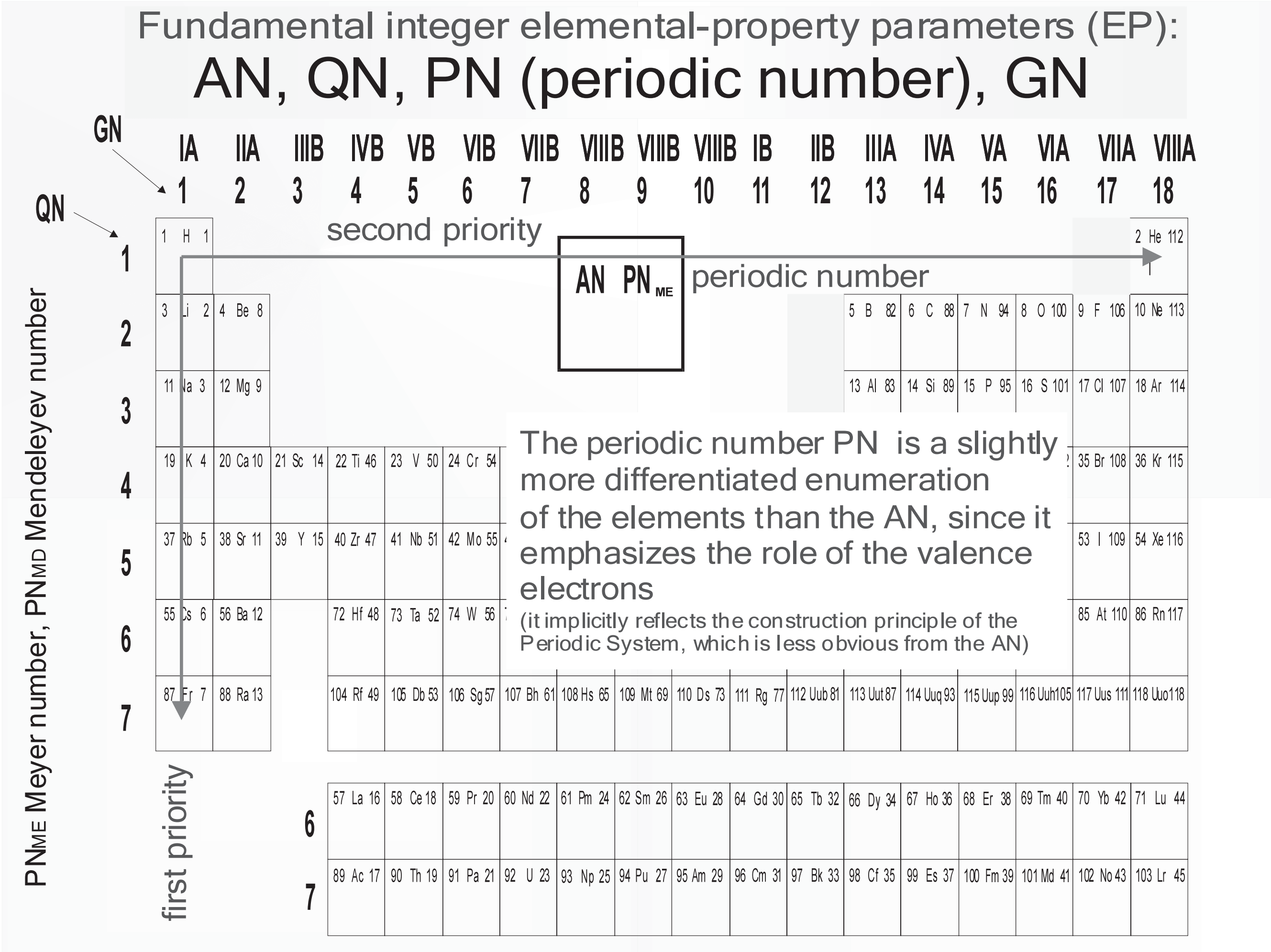




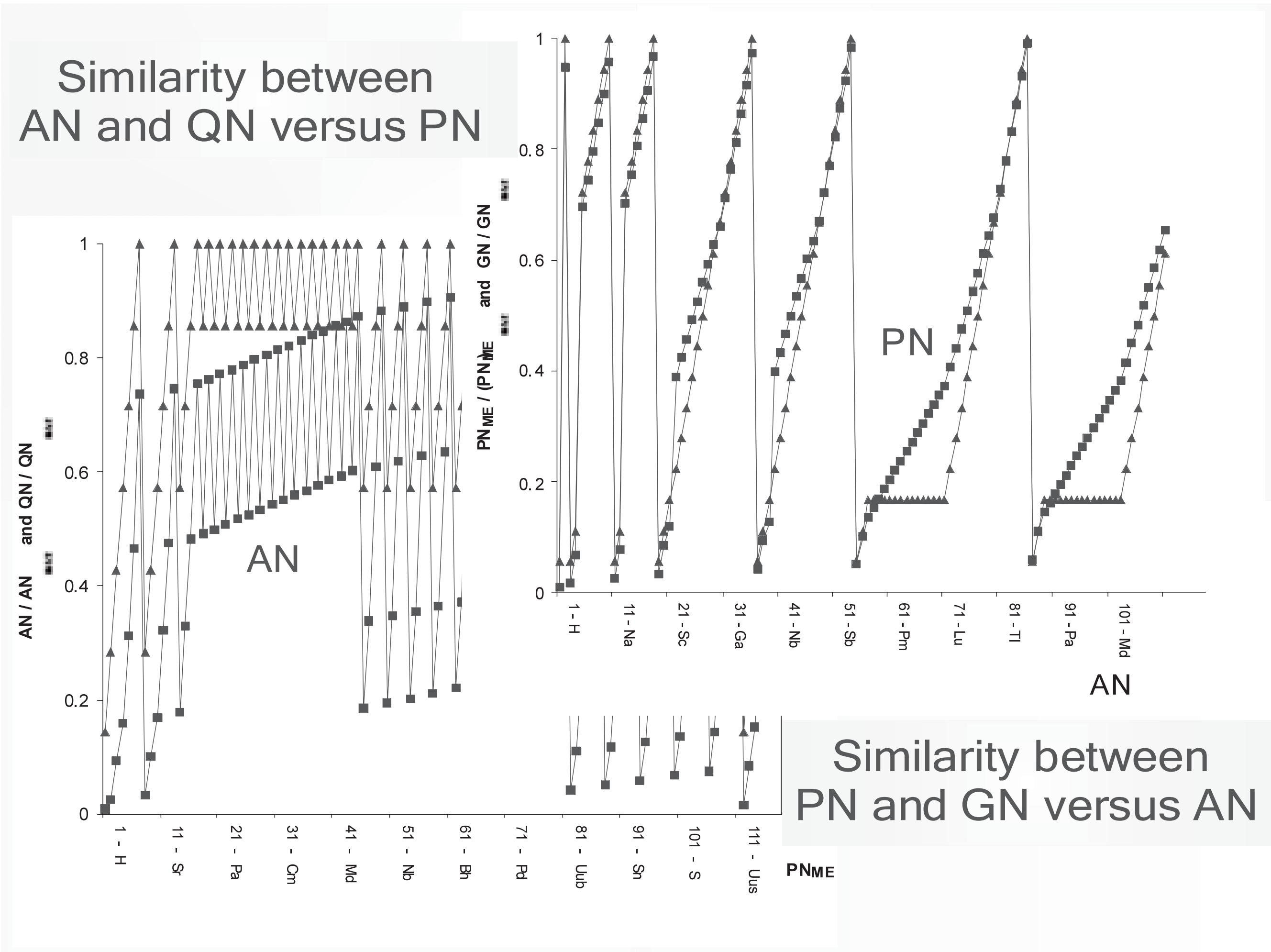
Available compilation of crystallographic data and phase diagram


Conclusions: No possible chem. systems vs. No. experimental facts (Materials DB)
NO MAJOR 'stable' EFFORTS WORLDWIDE will lead to 'BOTTLENECK'
Materials Databases
published experimental and calculated facts
distinct phases level
Elemental-Property Parameter Databases
experimental and calculated
No. of chemical systems vs. No. of experimental facts (Materials DB)
Materials Databases
strategically (large scale) calculated facts from first principles calculations
Materials Databases
own calculated facts from first principles calculations
Materials Databases
Elemental-Property Parameter - Materials Property Correlations (by users)


Pattern by linking elemental-property parameters and Materials Properties
(leading to Prediction Ability)
Chemical Potential after Miedema
Miedema Plot
compound formation
non-compound formation
Prediction?
Materials Property
elemental-property parameter
0
0.5
1.0
1
2
3
4



Fundamental integer elemental-property parameters (EP):
AN, QN, PN (periodic number), GN
GN
QN
IA IIA IIIB IVB VB VIB VIIB VIIIB VIIIB VIIIB IB IIB IIIA IVA VA VIA VIIA VIIIA
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18
1 2 3 4 5 6 7
second priority
AN PNME
periodic number
first priority
PNME Meyer number, PNMD Mendeleyev number
1 H 1
2 He 112
3 Li 2 | 4 Be 8 | 5 B 82 | 6 C 88 | 7 N 94 | 8 O 100 | 9 F 106 | 10 Ne 113
11 Na 3 | 12 Mg 9 | 13 Al 83 | 14 Si 89 | 15 P 95 | 16 S 101 | 17 Cl 107 | 18 Ar 114
19 K 4 | 20 Ca 10 | 21 Sc 14 | 22 Ti 46 | 23 V 50 | 24 Cr 54 | 35 Br 108 | 36 Kr 115
37 Rb 5 | 38 Sr 11 | 39 Y 15 | 40 Zr 47 | 41 Nb 51 | 42 Mo 55 | 53 I 109 | 54 Xe 116
55 Cs 6 | 56 Ba 12 | 72 Hf 48 | 73 Ta 52 | 74 W 56 | 85 At 110 | 86 Rn 117
87 Fr 7 | 88 Ra 13 | 104 Rf 49 | 105 Db 53 | 106 Sg 57 | 107 Bh 61 | 108 Hs 65 | 109 Mt 69 | 110 Ds 73 | 111 Rg 77 | 112 Uub 81 | 113 Uut 87 | 114 Uuq 93 | 115 Uup 99 | 116 Uuh 105 | 117 Uus 111 | 118 Uuo 118
6: 57 La 16 | 58 Ce 18 | 59 Pr 20 | 60 Nd 22 | 61 Pm 24 | 62 Sm 26 | 63 Eu 28 | 64 Gd 30 | 65 Tb 32 | 66 Dy 34 | 67 Ho 36 | 68 Er 38 | 69 Tm 40 | 70 Yb 42 | 71 Lu 44
7: 89 Ac 17 | 90 Th 19 | 91 Pa 21 | 92 U 23 | 93 Np 25 | 94 Pu 27 | 95 Am 29 | 96 Cm 31 | 97 Bk 33 | 98 Cf 35 | 99 Es 37 | 100 Fm 39 | 101 Md 41 | 102 No 43 | 103 Lr 45
The periodic number PN is a slightly more differentiated enumeration of the elements than the AN, since it emphasizes the role of the valence electrons
(it implicitly reflects the construction principle of the Periodic System, which is less obvious from the AN)

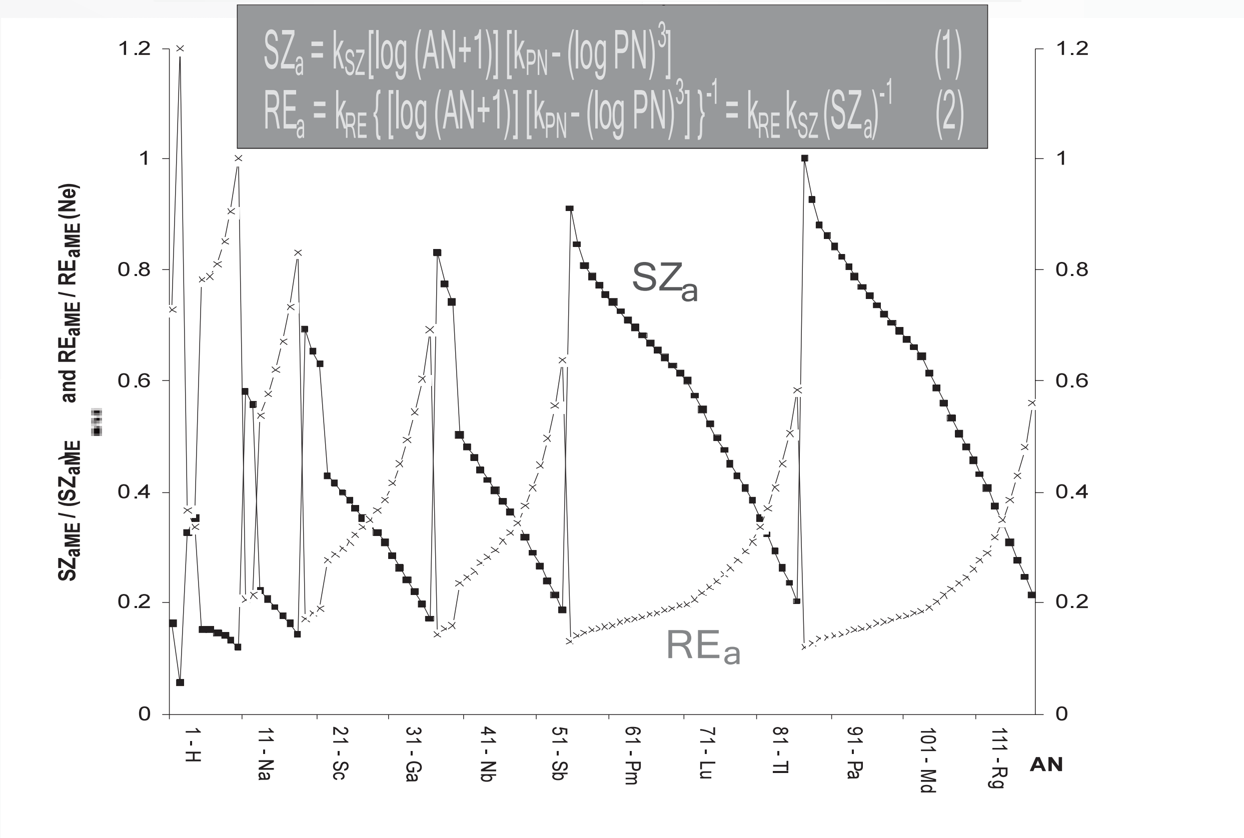


Similarity between AN and QN versus PN
AN / AN and QN / QN
AN
1 - H
11 - Sr
21 - Pa
31 - Cm
41 - Md
51 - Nb
61 - Bh
71 - Pd
81 - Uub
91 - Sn
101 - S
111 - Uus
PNME
PNME / (PNME and GN / GN
PN
1 - H
11 - Na
21 - Sc
31 - Ga
41 - Nb
51 - Sb
61 - Pm
71 - Lu
81 - Tl
91 - Pa
101 - Md
AN
Similarity between PN and GN versus AN

Non-integer elemental-property parameters Atomic Size SZa + Atomic Reactivity REa approximated as functions of AN and PN (plotted vs. AN)

$$SZ_a = k_{SZ}[\log(AN+1)]\,[k_{PN} - (\log PN)^3] \qquad (1)$$

$$RE_a = k_{RE}\{[\log(AN+1)]\,[k_{PN} - (\log PN)^3]\}^{-1} = k_{RE}\,k_{SZ}\,(SZ_a)^{-1} \qquad (2)$$



Conclusions Elemental-property parameters

1) An adequate description of the derived elemental-property parameters requires the introduction of the periodic number PN in addition to the well-established atomic number AN.

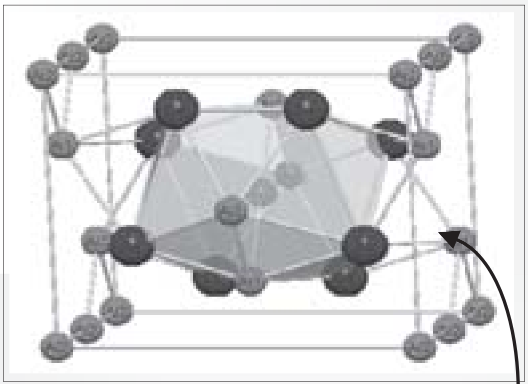
2) The derived elemental-property parameters atomic size SZ_a, and its reciprocal the atomic reactivity RE_a can be expressed as functions of AN and PN. Other elemental-property parameter functions, like the mass density can be described by combination of functions belonging to one or more pattern groups.

3) The result of equation (2): $RE_a = k_{SZ}\,k_{RE}\,(SZ_a)^{-1}$ is most outstanding. ⇨ The atomic reactivity RE_a (different electronegativity scales belong to this pattern group) of an element is the reciprocal value of its atomic size SZ_a

4) We argue that all elemental-property parameter patterns can be derived from AN and PN

Method to link Elemental-property parameters (expressions) with Materials Property

					3.45	4.20
25	Fe 26	Co 27	Ni 28	Cu 29	Zn 30	Ga 3
5	4.93	5.10	5.20	4.45	4.10	4.10
43	Ru 44	Rh 45	Pd 46	Ag 47	Cd 48	In 49
0	5.40	5.40	5.45	4.35	4.05	3.90
75	Os 76	Ir 77	Pt 78	Au 79	Hg 80	Tl 81
0	5.40	5.55	5.65	5.15	4.20	3.90



elemental-property parameters EP + Math.Operators

e.g.

- Atomic Number AN
- Melting Temperature
- Electronegativity
- Group Number GN
- Periodic Number PN
- Pseudopotential Radi
- ......

elemental-property parameter expression

Sum: EP(A) + EP(B)
Difference: IEP(A) - EP(B)I
Ratio: EP(A)/EP(B)
Product: EP(A)*EP(B)
Maximum: Max(EP(A), EP(B))
Minimum: Min(EP(A), EP(B))

Math.Operators e.g.

- Sum
- Difference
- Ratio
- Product
- Maximum
- Minimum
- .....

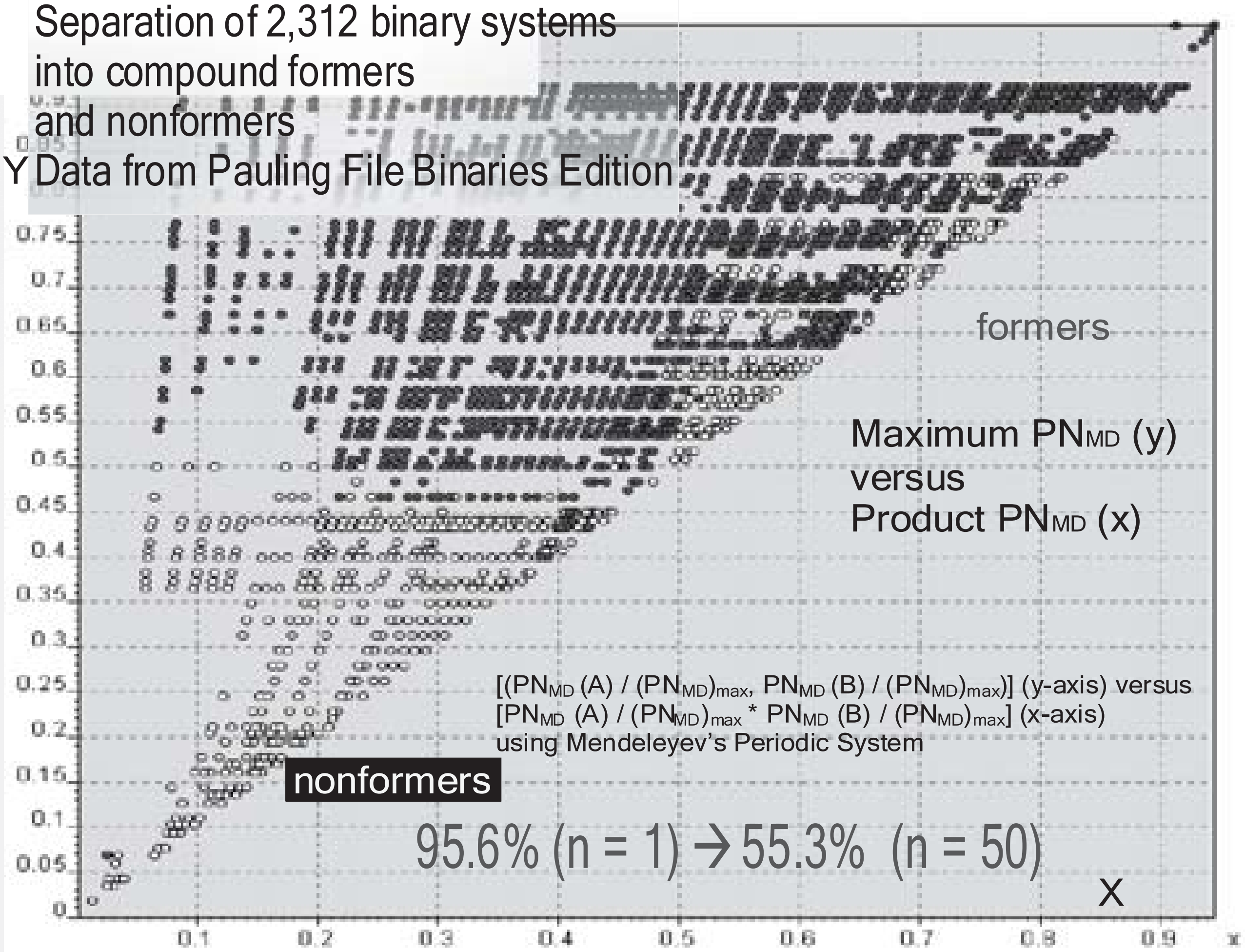
Materials Property

used as axes in a EPE - Materials Property plot

x-axes: Difference: EP(A) - EP(B) Electronegativity
y-axes: Difference: EP(A) - EP(B) Pseudopotential Radi
z-axes: Sum: EP(A) + EP(B) Group Number

Separation of 2,312 binary systems into compound formers and nonformers

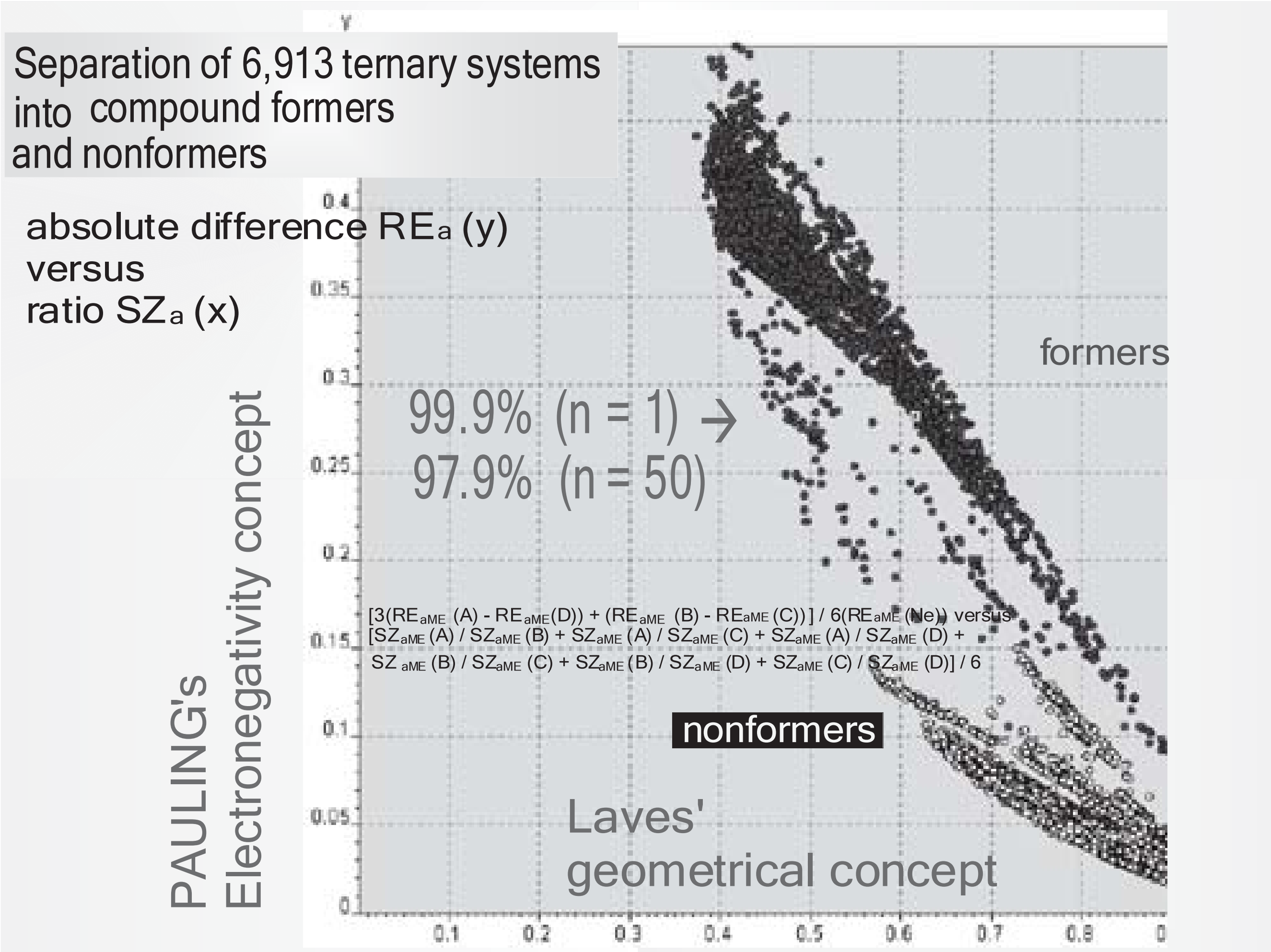
Data from Pauling File Binaries Edition



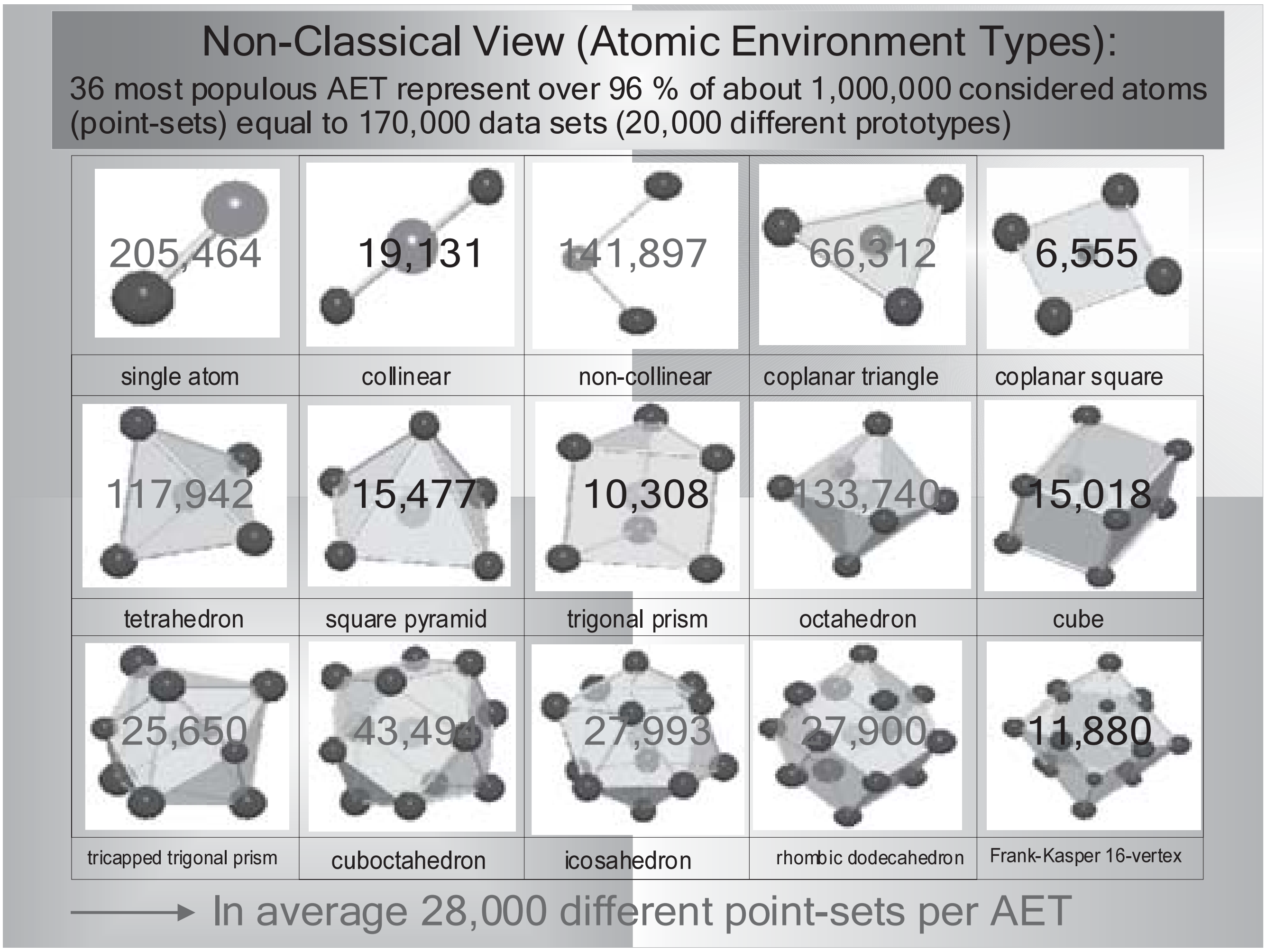
Maximum PN_{MD} (y) versus Product PN_{MD} (x)

$[(PN_{MD}(A) / (PN_{MD})_{max}, PN_{MD}(B) / (PN_{MD})_{max})]$ (y-axis) versus $[PN_{MD}(A) / (PN_{MD})_{max} * PN_{MD}(B) / (PN_{MD})_{max}]$ (x-axis) using Mendeleyev's Periodic System

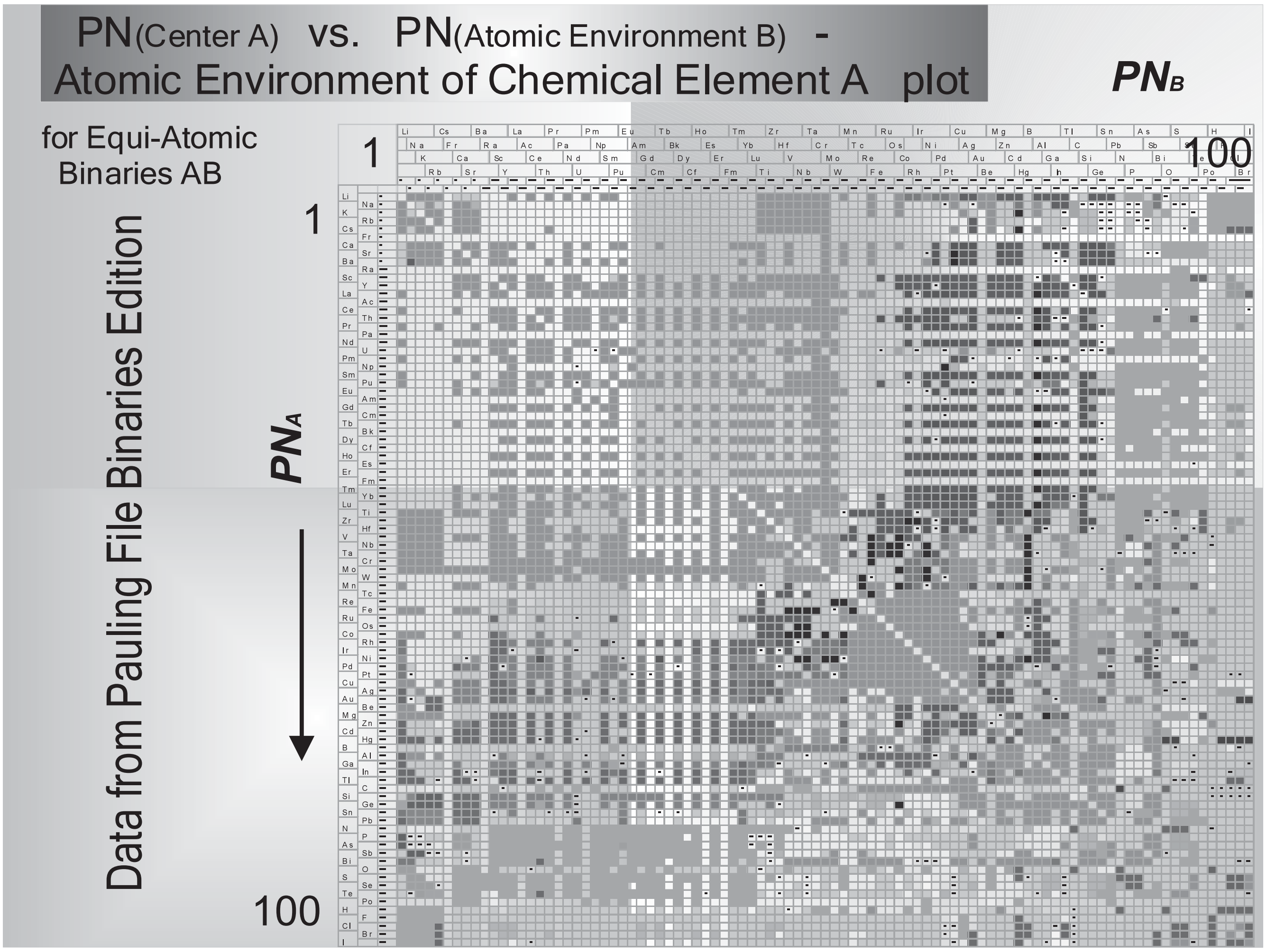
95.6% (n = 1) → 55.3% (n = 50)

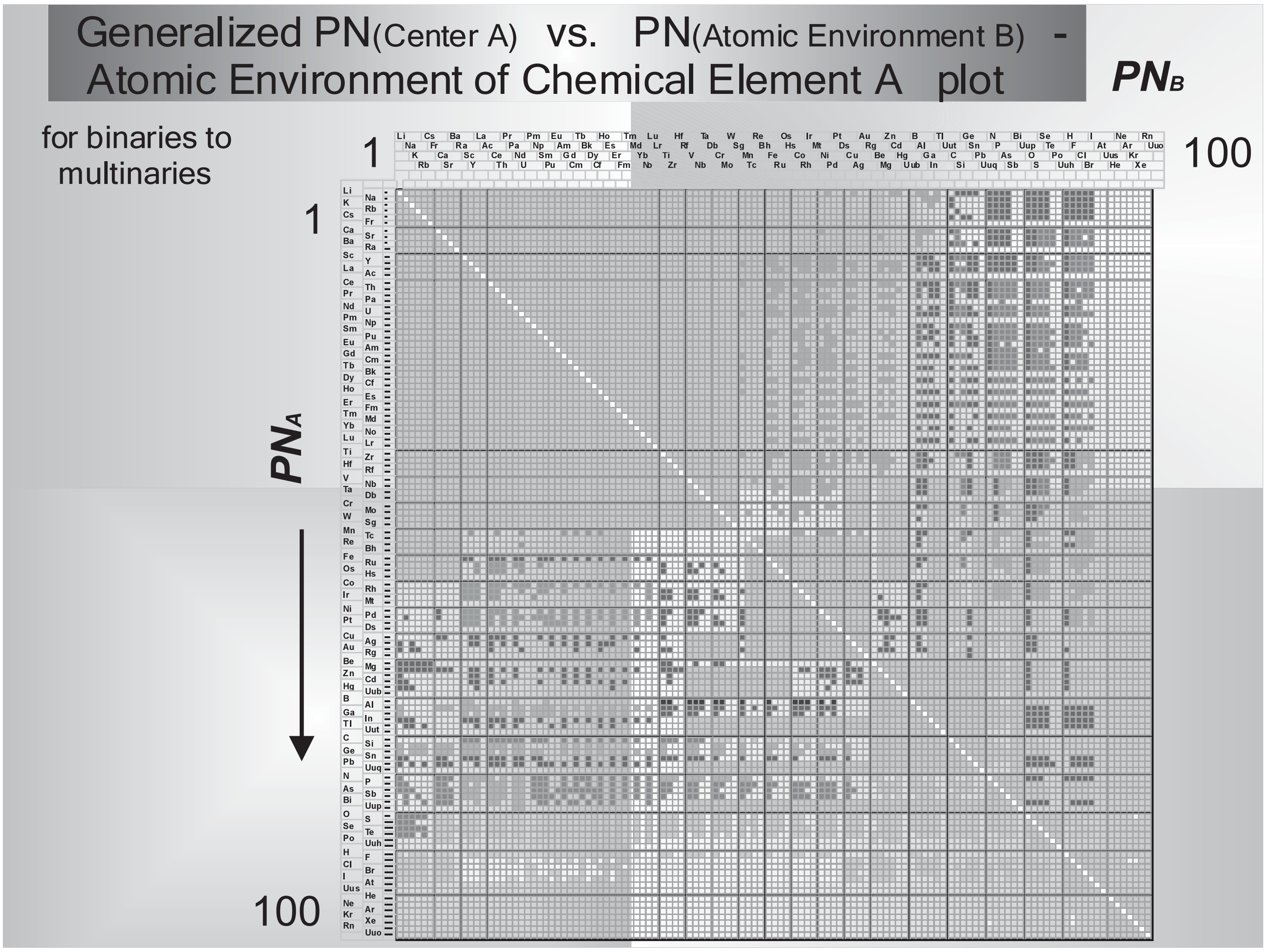


Separation of 6,913 ternary systems
into compound formers
and nonformers
absolute difference REa (y)
versus
ratio SZa (x)
PAULING's
Electronegativity concept
99.9% (n = 1) →
97.9% (n = 50)
formers
[3(REaME (A) - REaME(D)) + (REaME (B) - REaME (C))] / 6(REaME (Ne)) versus
[SZaME (A) / SZaME (B) + SZaME (A) / SZaME (C) + SZaME (A) / SZaME (D) +
SZ aME (B) / SZaME (C) + SZaME (B) / SZaME (D) + SZaME (C) / SZaME (D)] / 6
nonformers
Laves'
geometrical concept
y
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8



Non-Classical View (Atomic Environment Types):
36 most populous AET represent over 96 % of about 1,000,000 considered atoms
(point-sets) equal to 170,000 data sets (20,000 different prototypes)
205,464
single atom
19,131
collinear
141,897
non-collinear
66,312
coplanar triangle
6,555
coplanar square
117,942
tetrahedron
15,477
square pyramid
10,308
trigonal prism
133,740
octahedron
15,018
cube
25,650
tricapped trigonal prism
43,494
cuboctahedron
27,993
icosahedron
27,900
rhombic dodecahedron
11,880
Frank-Kasper 16-vertex
In average 28,000 different point-sets per AET


PN(Center A) vs. PN(Atomic Environment B) -
Atomic Environment of Chemical Element A plot
for Equi-Atomic Binaries AB
Data from Pauling File Binaries Edition
PNB
PNA
1
100
1
100

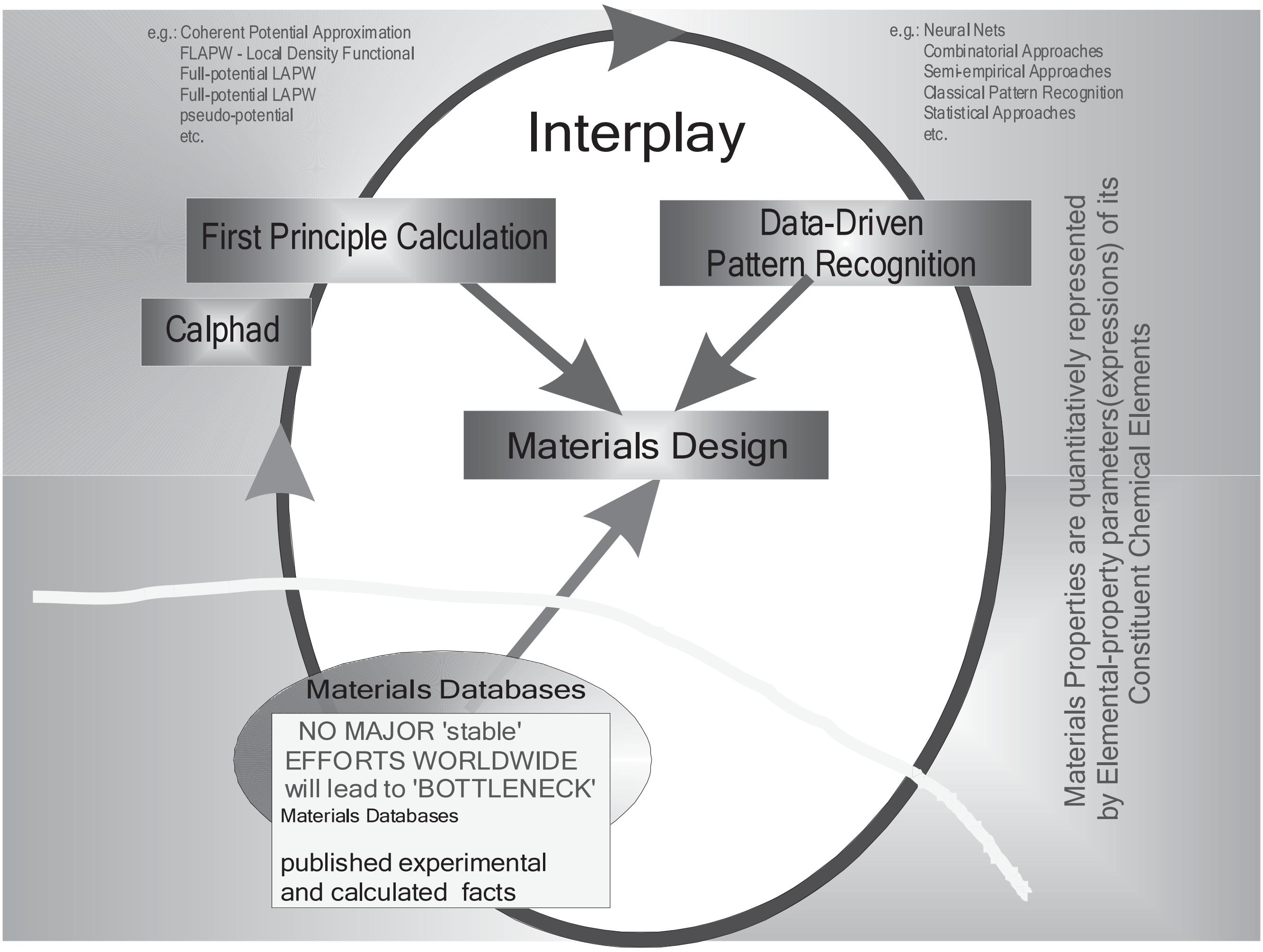

Generalized PN(Center A) vs. PN(Atomic Environment B) -
Atomic Environment of Chemical Element A plot
for binaries to multinaries
PNB
PNA
1
100
1
100

Conclusions: Elemental-property parameters expressions - Materials property correlations

1) Materials Properties can be formulated as sole functions of AN and PN of its constituent chemical elements, respectively defined functions of AN and PN, such as the atomic size SZ_a(AN,PN), the atomic reactivity RE_a(AN,PN).

2) Constituent Chemical elements (AN, PN) - Materials Properties correlations can be extended from Binaries to Ternaries, Quaternaries, ...

"Structure-sensitive material properties are quantitatively described by the elemental-property parameters EP: AN and PN (or simple mathematical functions of them) of the constituent chemical elements."



Finding Materials for Transformation Toughening through Datamining

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Transformation toughening is a highly effective self-healing mechanism that is used to enhance ductility in brittle materials where a volume expanding phase transformation of a dispersed phase is used to counteract stress concentration near a crack tip. In ceramics the transforming dispersion is usually zirconia, and in metallic materials martensitic phases are used.

A combination of concepts such as structure maps, classification indices such as Mendeleev numbers and atomic environment types, and tools such as structure databases [1], data mining and electronic density functional prediction of structural stability, are used to find new phases for transformation toughening dispersions.

The well-defined criteria that such candidate dispersoid materials must meet, such as undergoing a phase transformation under (inhomogeneous) stress associated with volume and/or crystallite shape change, as well as requiring no mass transport, will be discussed. Our process of refining materials criteria, and of applying these criteria will be outlined in the talk and some specific candidate dispersoid materials for transformation toughening will be analyzed.

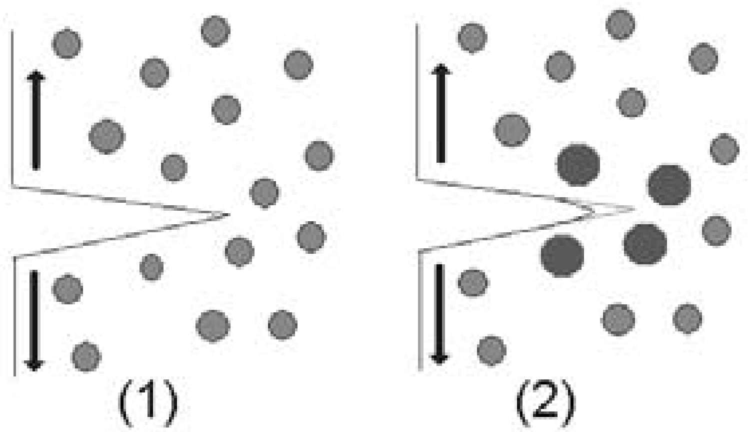

Figure 1. Principle of crack closure through transformation toughening: metastable dispersoids (red circles) transform under the stress field near the crack; transformed dispersoids (blue circles) expand and thereby close the crack

References

[1] P. Villars, M. Berndt, K. Brandenburg, K. Cenzual, J. Daams, F. Hulliger, T. Massalski, H. Okamoto, K. Osaki, A. Prince, H. Putz, S. Iwata, PAULING FILE CDROM, Binaries Edition, ASM International, Materials Park, OH, 2002

Inference from Various Material Properties Using Mutual Information and Clustering Methods

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Abstract

Mutual information and clustering methods [1] have become more and more popular with the increasing accessibility and availability of categorized data. Mutual information maps present a practical and quantitative way to infer about relations between various properties (or combination of properties) given that sufficient data are available. They may lead to previously unknown / unsuspected factors relating to the property being investigated. Clustering method also enables one to guess or at the very least decrease the number of possible candidates sought to have some specific properties. Bayesian inference methods in context with neural networks have been widely used in materials science through non-linear regression techniques for the refinement of known properties [2]. Currently, clustering and the mutual information maps methods are used mostly for structure prediction [3-6] and also to guess the possibility of a compound occurrence [7]. The studies so far have focused on the discrete parameters such as composition, atomic number factor, Mendeleev number. In this work, aside from discrete parameters, by means of a probability binning algorithm [8] originally proposed for cytometry applications, we also study the correlation of continuous parameters. Pauling File [9] was used for data acquisition.

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[1] D.J.C. MacKay, "Information Theory, Inference and Learning Algorithms" Cambridge University Press, 2005 UK.

[2] H.K.D.H. Bhadeshia, ISIJ Int. 39, 966 (1999).

[3] C.C. Fischer, K.J. Tibbetts, D. Morgan and G. Ceder, Nature Mater. 5, 641 (2006).

[4] G. Ceder, D. Morgan, C.Fischer, K. Tibbetts and S. Curtarolo, MRS Bull. 31, 981 (2006).

[5] D. Morgan, J. Rodgers and G. Ceder, J. Phys.: Condens. Matter 15, 4361 (2003).

[6] P. Villars, K. Cenzual, J. Daams, Y. Chen and S. Iwata, J. Alloy Compd. 367 167 (2004).

[7] P. Villars, K. Brandenburg, M. Berndt, S. LeClair, A. Jackson, Y.-H. Pao, B. Igelnik, M. Oxley, B. Bakshi, P. Chen and S. Iwata, J. Alloy Compd. 317-318 26 (2001).

[8] M. Roedereri A. Treister, W. Moore and L.A. Herzenberg, Cytometry 45 37 (2001).

[9] P. Villars, M. Berndt, K. Brandenburg, K. Cenzual, J. Daams, F. Hulliger, T. Massalski, H. Okamoto, K. Osaki, A. Prince, H. Putz, S. Iwata, PAULING FILE CDROM, Binaries Edition, ASM International, Materials Park, OH, 2002 USA

Inference from Various Material Properties Using Mutual Information and Clustering Methods

MITS 2008

Emre S. Tasci & Marcel H. F. Sluiter

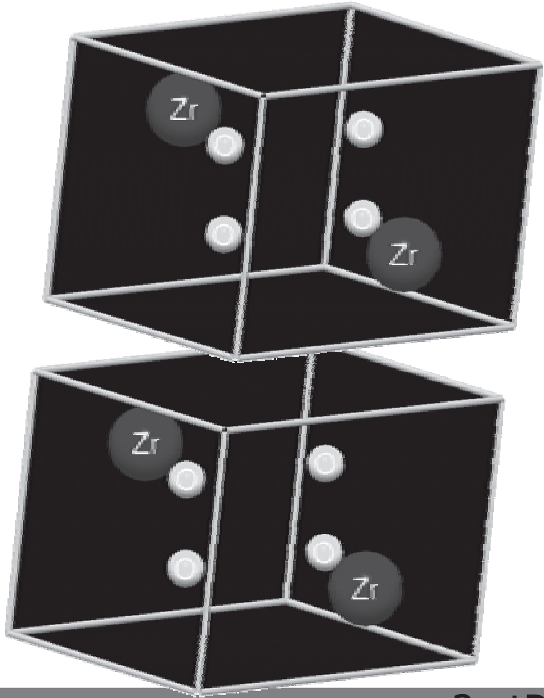
July 17, 2008

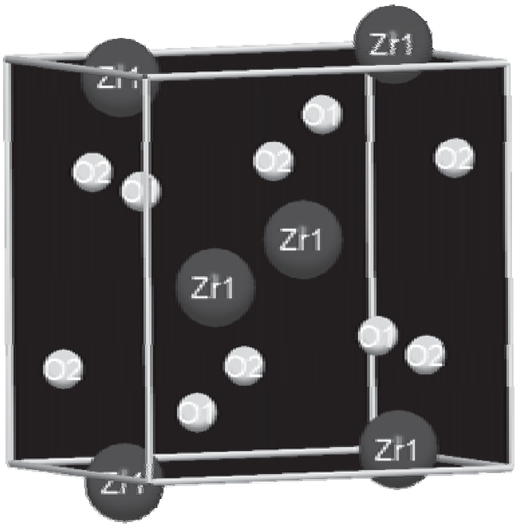
The Situation

- R.C. Garvie and his collaborators, in their "Ceramic Steel?" titled article reported the existence of the metastable tetragonal zirconia at room temperature.

Garvie R.C et al., Nature 1975 **258** 703-4

The Situation





2x tP6 -> mP12

0.1398 nm³ -> 0.1403 nm³

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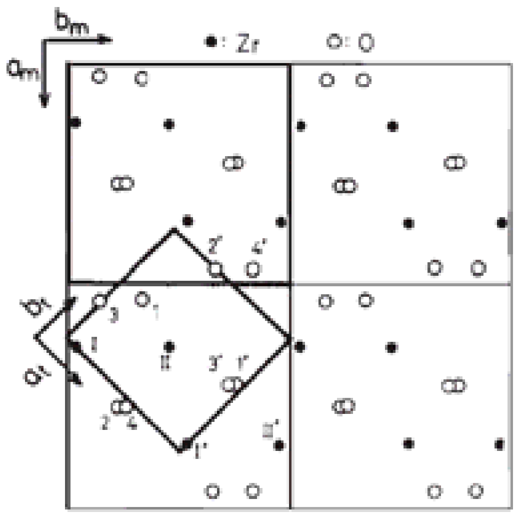
t->m transformation



Negita K., Takao H., J. Phys. Chem. Sol. 1989 **50** 325-31

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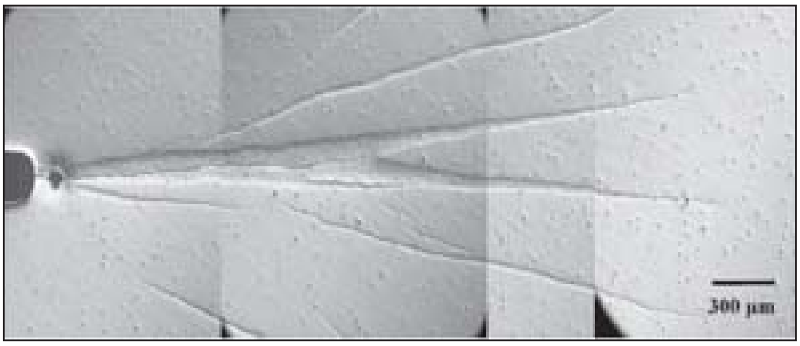
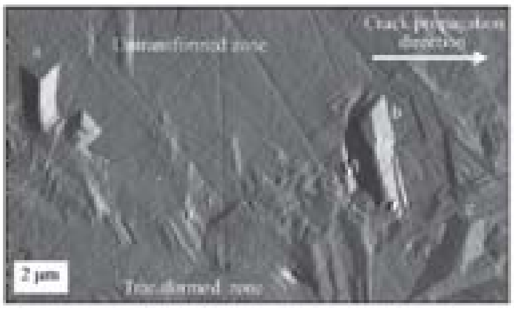
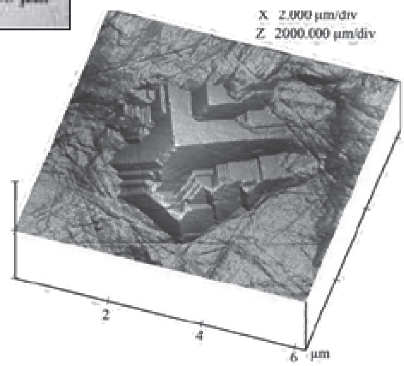
The Situation







Deville S. et al., J. Eur. Ceram. Soc. 2005 **25** 3089-96
El Attaoui H., J. Eur. Ceram. Soc. 2007 **27** 483-6

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The Problem

- ZrO_2 is expensive.
- Can’t wait for another “accident” to find alternatives.

- (And also, it would be good if we could have similar behaviour for high/low temperature applications.)

Clues

- Focus on the Oxides.
- The transformation should be diffusionless:
  - There must be a metastable phase present in the material.
  - Transformation is virtually instantaneous and does not require time-dependent process.
  - The composition must be preserved
  - It must be associated with a change in shape/volume (stress inducement).

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Validation

- Just consider –allowed- transitions from the higher to lower orders of symmetry with respect to parent – child hierarchy.
- Check the temperature/pressure conditions of the data acquired.

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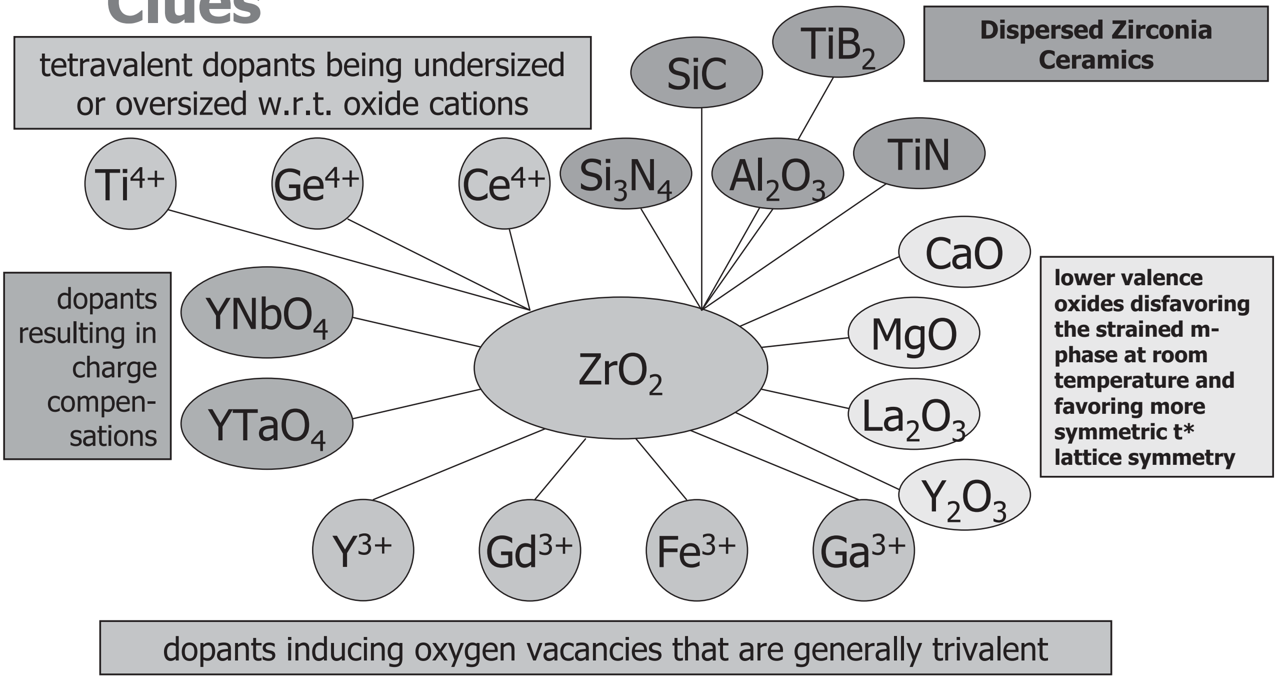
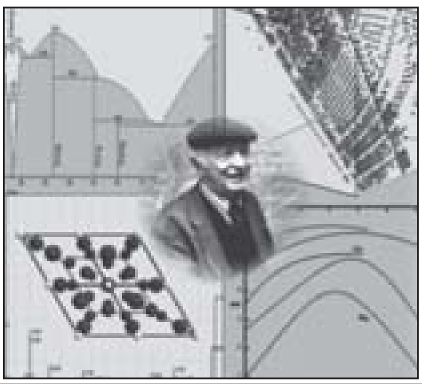
Clues



Methods : Clustering

- How are all these elements related? What do they have in common with ZrO_2? What are the other materials that also interact with these elements?

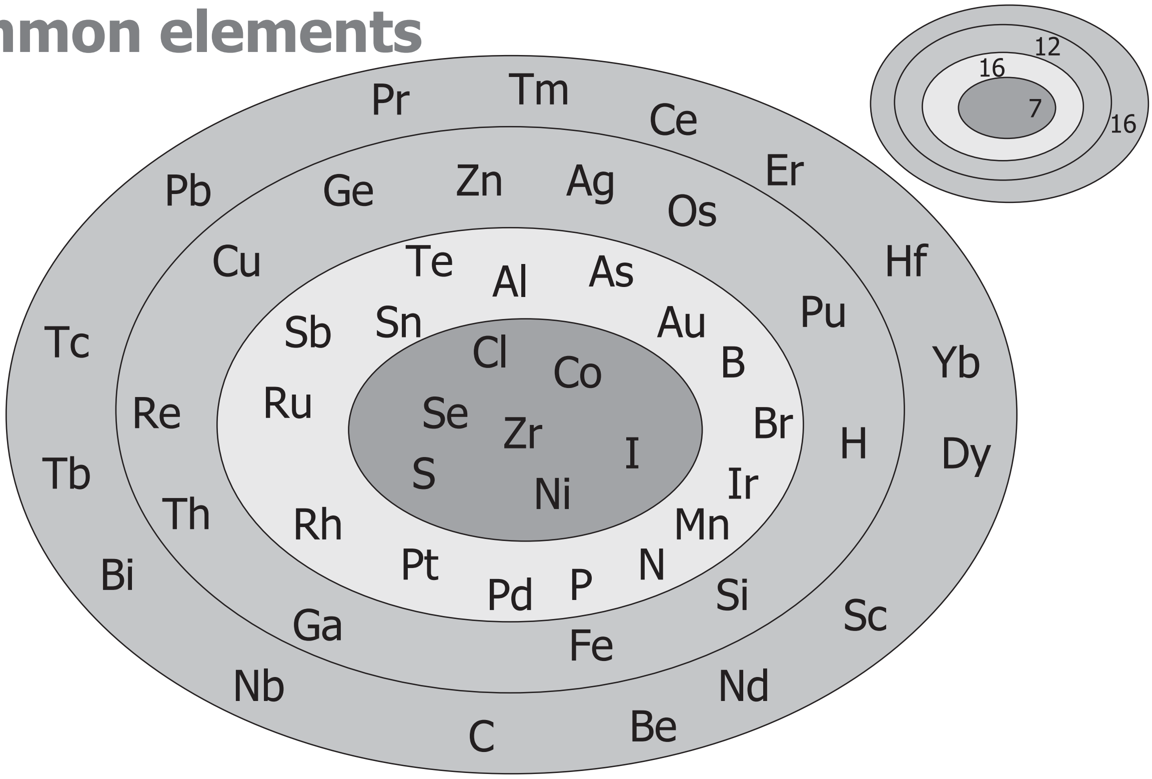


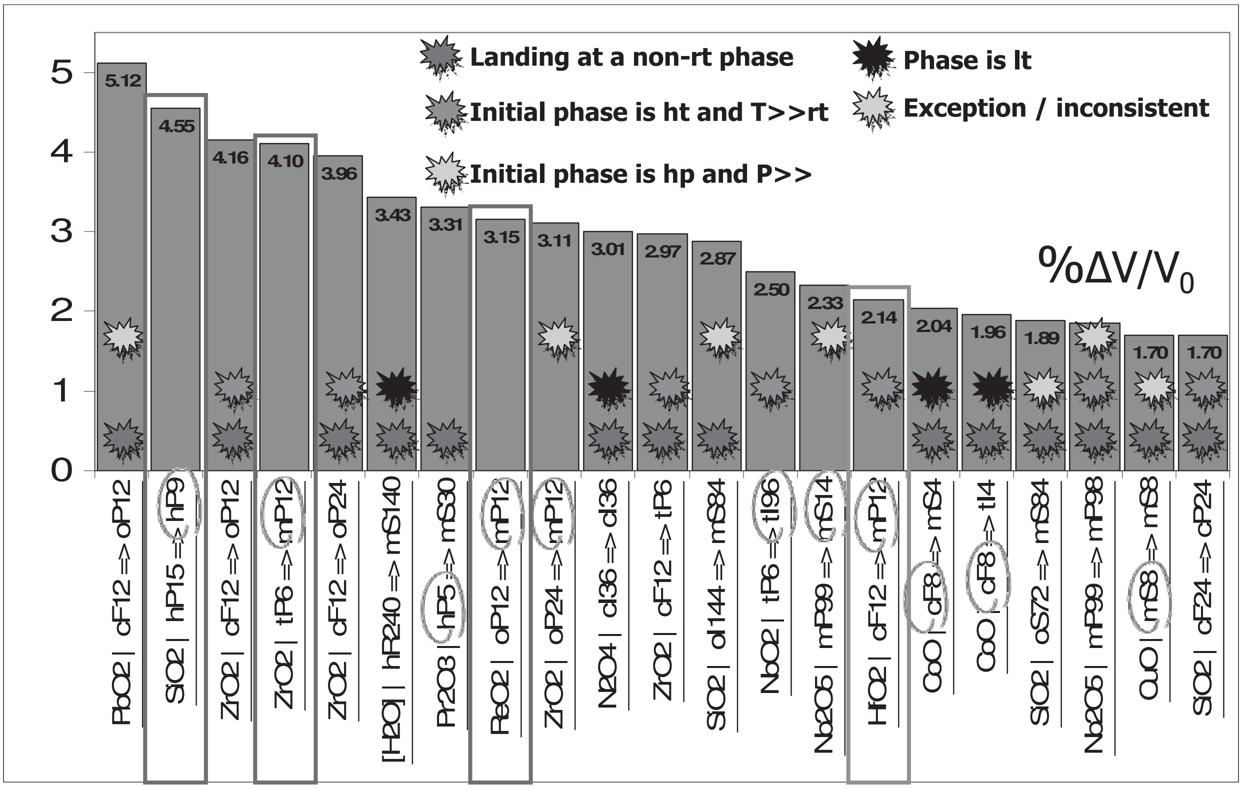
PAULING FILE

Inorganic Materials Database and Design System

Edited by P. Villars (editor-in-chief),
K. Cenzual, J. Daams, F. Hulliger, H. Okamoto, K. Osaki, A. Prince
S. Iwata (project coordination)

Common elements





Conclusions

- Simple clustering narrowed down the pool.
- Employing group theory for filtering is very effective.
- Two candidates for TT at ambient temperature.
- Much more for high/low temperatures.
- The results should always be eye-balled.

- Dopants for (meta-)stabilizing should also be looked for.

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Proposal of the XML Specification as a Standard for Materials Database Query Submission and Result Retrieval

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* Corresponding author's e-mail address: e.tasci@tudelft.nl

Abstract

Due to the continuing advance in information gathering, parsing and categorization techniques, as well as progress in communications, data availability and accessibility, the applications of information theory in the materials science are becoming common practice. With respect to different organizations and classifications, many materials databases (spanning common or distinct material types) have been constructed with different interfaces and as one would expect, different processing mechanisms.

The inner mechanisms of the database querying is -most of the time- irrelevant to the common user since one does not need to know how the data related to his query is being fetched. Alas, we can not say the same thing about the interfaces used both in query submission and result retrieval. A query consists of two sets of parameters (**A | B**) where **B** = $\{b_i\}$ represents the conditions the sought object(s) should fulfill while **A** = $\{a_j\}$ represents the properties to be acquired belonging to the sought object(s). Although using interfaces provide an easy and practical way for query submission, it seriously hinders systematic querying (i.e., by means of a computer code). The same is valid for the retrieved result listing.

Different schemes for standardization of specific categorical properties have been proposed before like the CIF [1] for crystallography classification or PDF [2] for diffraction classification. By proposing the Extensible Markup Language (XML) [3], a fee-free standard specification developed by the World Wide Web Consortium, to be used as the standard for materials database querying and retrieval, we hope that it will be possible to use one written code to query and retrieve data from any materials database without modifying the code, also benefit from easily performed automated queries in addition being able to cover different branches in material sciences. There is already a tailored XML schema MatML [4], prepared for materials scientific purposes which can be expanded and developed further to cover also database related properties but also a new schema from scratch is also possible and doable. Usage of XML does not conflict with the currently ongoing access restrictions and usage limitations imposed by the database maintainers since it is only a new means for input/output formatting. Being a universally accepted standard specification, XML is supported by all of the common programming languages meaning readily coded applications and libraries for all major platforms.

References

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[3] World Wide Web Consortium, Extensible Markup Language 1.1, 2nd Ed.,

http://www.w3.org/TR/xml11/ (2006).

[4] MatML Coordination Committee, http://www.matml.org (2005).

Proposal of the XML Specification as a Standard for Materials Database Query and Result Retrieval

MITS 2008

Emre Tasci

July 10, 2008

TU Delft
Delft University of Technology

Current situation

- Different materials databases for different aspects.
- They span many common properties.
- In order to query them, one should use the provided interface / specific input script.
- The result is also fetched in a db-specific format.

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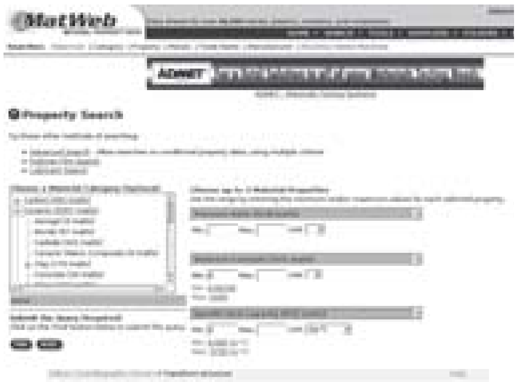

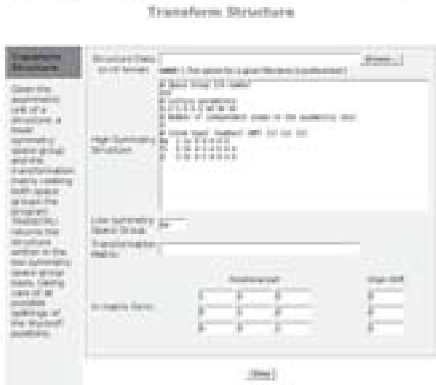

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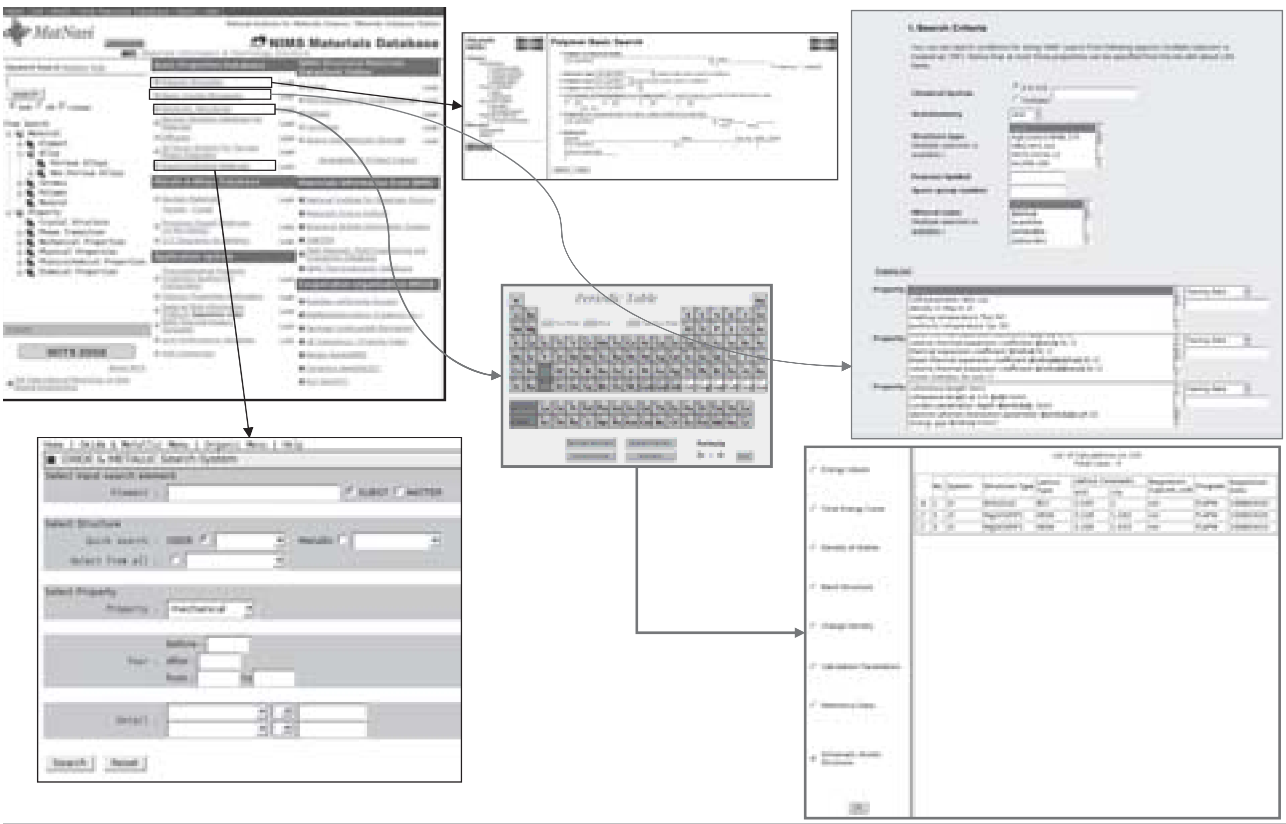

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"One format to bind them all"

- eXtensible Markup Language (XML)
- Easy to read, parse and implement
- Already the standard for many fields
- Readily supported by programming languages

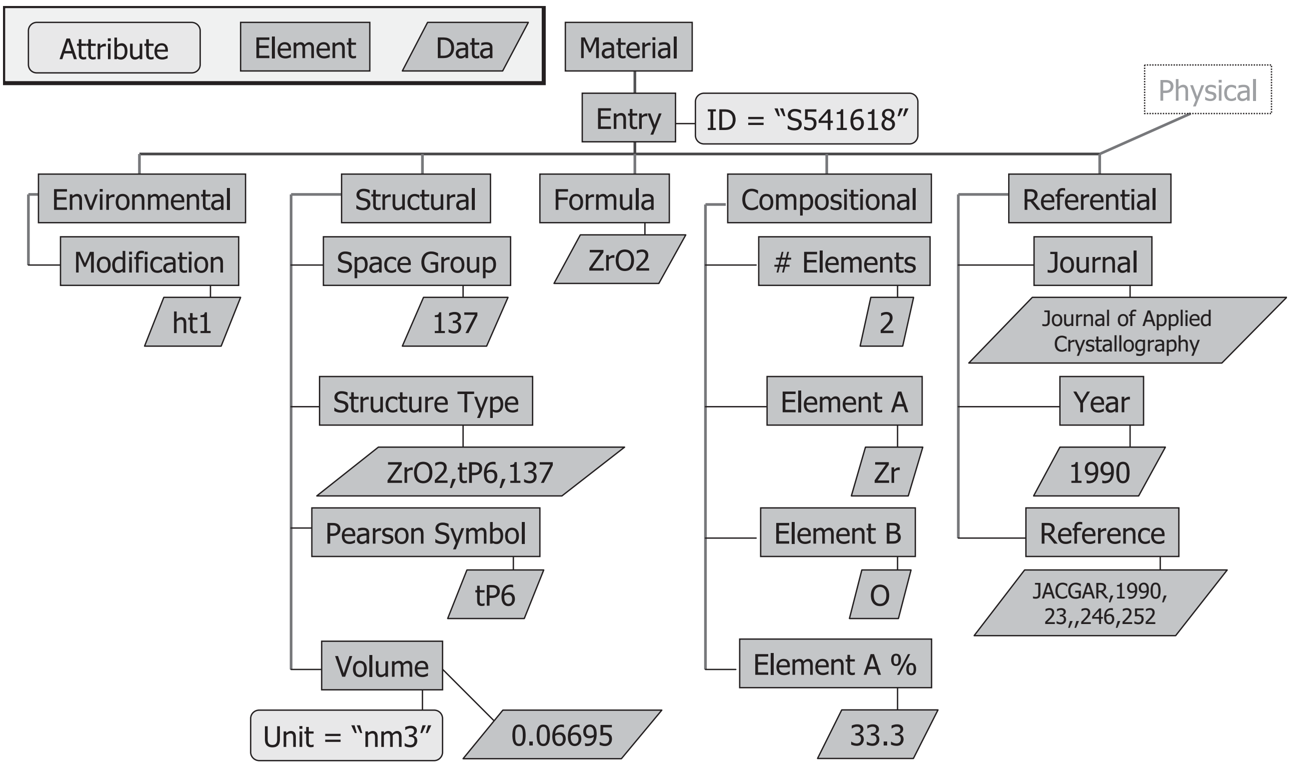
about XML...

- Designed to carry data, not to display data
- Designed to be self-descriptive
- Does not *DO* anything – it's just pure information.
- It is plain text – readable for on the spot checks
- It is extensible – full compatability

- It is a software and hardware independent tool for carrying information

XML Example

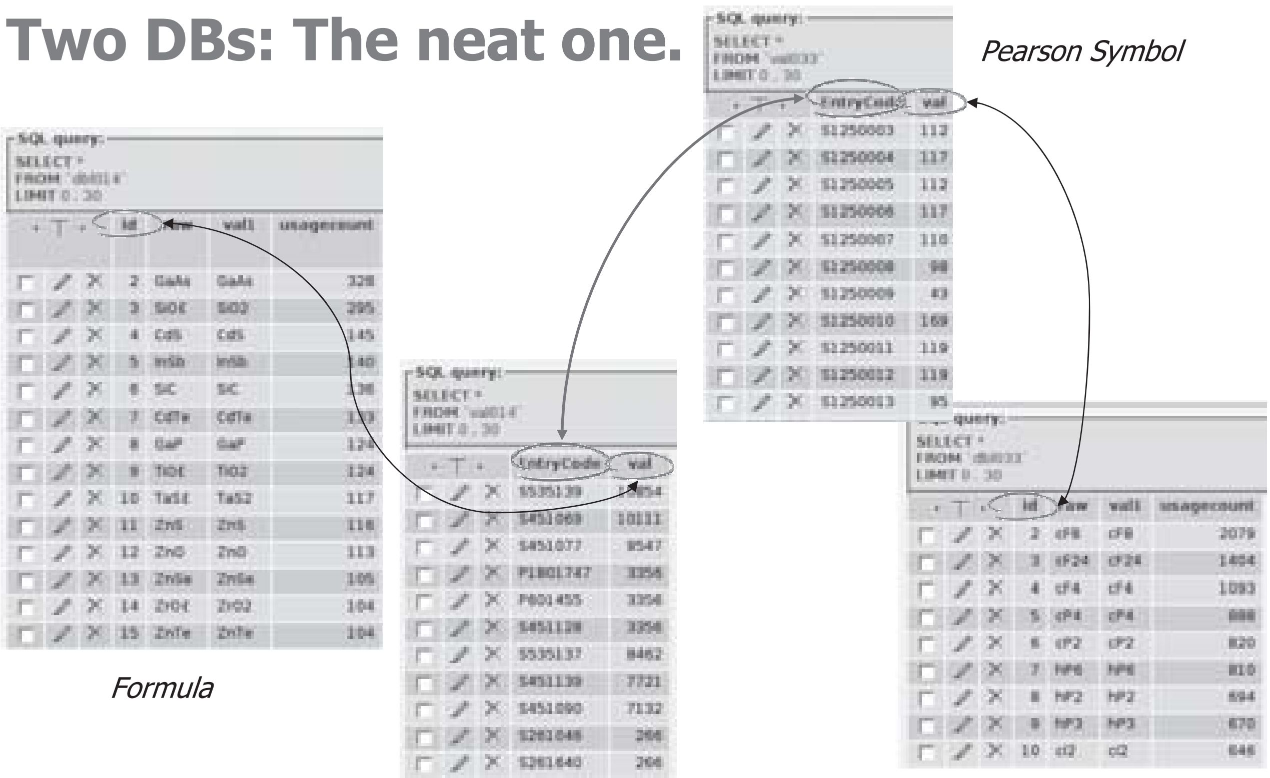
- Formula : ZrO2
- Modification : ht1
- Crystal System : tetragonal
- Pearson Symbol : tP6
- Cell Volume : 0.06695nm3
- Volume per atom : 0.0111583nm3
- Structure Type : ZrO2, tP6, 137
- Journal : Journal of Applied Crystallography
- Journal Abbr. : J. App. Cryst.
- Year : 1990
- Vol : 23
- First Page : 246
- Last Page : 252
- Reference : JACGAR, 1990, 23, ,246
- Authors : L. Lutterotti, P. Scardi



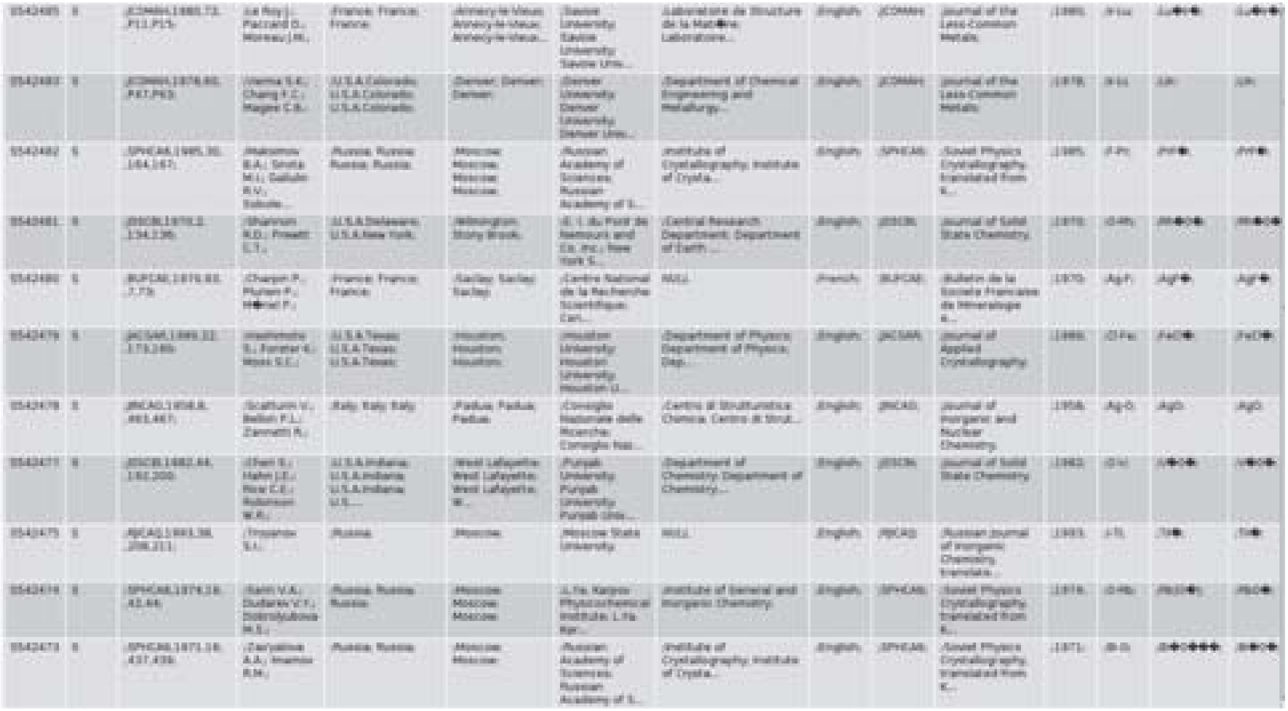
Sample


```xml
<material>
  <entry ID="S541618">
    <formula>
      <value>ZrO2</value>
    </formula>
    <environmental>
      <modification>ht1</modification>
    </environmental>
    <structural>
      <space_group>137</space_group>
      <structure_type>ZrO2,tP6,137</structure_type>
      <pearson_symbol>tP6</pearson_symbol>
      <volume unit="nm3">0.6695</volume>
    </structural>
    <compositional>
      <no_elements>2</no_elements>
      <element_A>Zr</element_A>
      <element_B>O</element_B>
      <element_A_per>33.3</element_A_per>
    </compositional>
    <referential>
      <journal_name>Journal of Applied Crystallography</journal_name>
      <year>1990</year>
      <reference>JACGAR,1990,23,,246,252</reference>
      <page_first>246</page_first>
      <vol>23</vol>
    </referential>
  </entry>
</material>
```


Two DBs: The neat one.



Two DBs: The “other” one..



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Demonstration...

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Conclusion

- XML is an efficient way to exchange data.
- It is easily implementable & extensible.
- Overcomes the boundaries between hardware & software.
- Already has a wide range of support.

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