International Conference of Materials Databases

Organized by
Materials Information Technology Station (MITS)
National Institute for Materials Science (NIMS)

Venue
Toshi Center Hotel
2–4–1, Hirakawacho Chiyodaku, Tokyo, Japan
MITS meeting 2006
International Conference of Materials Databases
Friday, January 20th, 2006
Venue:Toshi Center Hotel

Chairperson  Prof. Shuichi Iwata,  The University of Tokyo

9:00  Opening Remarks
Prof. Teruo Kishi,  President of NIMS

<Knowledge Discovery from Materials Databases>
9:10  Data Mining of Databases ................................................................. 1
Prof. Krishna Rajan,  Iowa State University
9:50  XML-based Data Management for Combinatorial Materials Science .......... 20
Prof. Mikk Lippmaa,  The University of Tokyo
10:30  Data/Modeling Driven Approach Towards Materials Design ..................... 38
Prof. Ying Chen,  The University of Tokyo
11:10  Development of Materials Risk Information Platform ............................. 51
Dr. Koichi Yagi,  NIMS

11:50 – 13:10    Lunch

<Business Model of Material Databases>
Chairperson  Prof. Yoshio Monma,  Kochi University of Technology
13:10  Introduction of Factual Databases in KISTI (Korea) .......................... 58
Dr. Sang-Ho LEE,  Korea Institute of Science and Technology Information
13:50  A Computer Matching Technique for Steel Grades Comparison between
Different Standards ......................................................................................... 84
Dr. Hang Su,  Central Iron and Steel Research Institute
14:30  Development of Optimum Material Selection Program for Various
Equipments .................................................................................................... 97
Dr. Shigemitsu Kihara,  Best Materia Co.

15:10 – 15:30  Coffee Break
Chairperson: Prof. Toshihiro Ashino, Toyo University

15:30 Material Selection Using Internet-Based Tools .................................................. 107
Dr. Dale O. Kipp, Automation Creations, Inc.

16:10 Landolt-Börnstein in the electronic age: the collection of “Numerical Data and Functional Relationships in Science and Technology” going online .......... 120
Dr. Rainer Poerschke, Springer Verlag GmbH

16:50 Closing Remarks
Dr. Koichi Yagi, NIMS

17:30 Reception
Data Mining of Databases

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1. Introduction

The search for new materials, whether through experiment or simulation has been a slow and arduous task, punctuated by infrequent and often unexpected discoveries. Each of these findings prompts a flurry of studies to better understand the underlying science governing the behavior of these materials. The few systematic efforts that have been made to analyze trends in data as a basis for predictions have in large part been inconclusive, not least of which is due to the lack of large amounts of organized data and even more importantly the challenge of sifting through them in a timely and efficient manner. When combined with a huge combinatorial space of chemistries as defined by even a small portion of the periodic table, it is clearly seen that searching for new materials with a tailored properties is a prohibitive task. Hence the search for new materials for new applications is limited to educated guesses. Data that does exist is often limited to small regions of compositional space. Experimental data is dispersed in the literature and computationally derived data is limited to a few systems for which reliable quantum mechanical information exists for calculations. Even with recent advances in high speed computing, there are limits to how many new alloys can be calculated. Hence this poses both a challenge and opportunity. The challenge is to both build and analyze extremely large disparate databases. It is here that data mining offers an opportunity to convert databases from static “search and retrieve” documents to a “computational laboratory” where patterns of behavior can be derived and “virtual” databases with new (and reliable data) can be established. In this presentation we provide examples of different data mining tools can be applied to databases to

2. What can we learn from data mining?

By integrating the mathematics of informatics tools into well organized databases, we can extract information to establish correlations between disparate and multivariate information across different length scales. We can probe large databases with multivariate and diverse information on thermophysical and thermochemical properties and identify critical chemistry-property correlations that otherwise would have been difficult to assess. Knowledge discovery in databases or data mining, an interdisciplinary field merging ideas from statistics, machine learning, databases, and parallel and distributed computing, provides a unique tool to integrate scientific information and theory for materials discovery. Data mining has been engendered by the phenomenal growth of data in all spheres of human endeavor, and the economic and scientific need to extract useful
information from the collected data. The key challenge in data mining is the extraction of knowledge and insight from massive databases. It takes the form of discovering new patterns or building models from a given dataset.

In this presentation we shall outline some of the challenges faced in data mining databases, including:

- **Missing Descriptors** – For a given predictive task, we would like to be able to exploit all relevant compounds even if some of the relevant descriptors are missing.

- **Skewed Responses** – To discover novel compounds with desired properties, we frequently would like to be able to predict properties in specific ranges that are precisely where we have the least amount of data. Available data tends to be highly skewed towards known compounds that possess this property to a measurable degree.

- **Incompleteness and Ambiguity of Data from Heterogeneous Sources** – For a specific property of interest (e.g. selectivity, structure etc.) heterogeneous data sources may introduce ambiguity in the representation of that property in the data. The experimentally measured activity may be reported using several metrics of varying quality, different descriptors may be used to measure similar properties, and a full set of properties will not be available for most compounds. The challenge is how to exploit all available data in these cases.

- **Large diverse set of potential descriptors** – Feature selection is essential since there are a large set of potential descriptors which may be irrelevant to the task at hand. This raises the issue of what descriptors are actually needed in a database.

3. **Summary**

To convert databases into knowledge discovery platform marks the next generation for the development of databases. In this presentation we will outline with some examples of different types of data mining tools and how they are applied to a diverse array of digital libraries in materials science. The framework for the development of an informatics infrastructure for materials science databases is also discussed.
DATA MINING of DATABASES

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Department of Materials Science & Eng.
Institute for Combinatorial Discovery
Iowa State University

MiTS  
TOKYO  
JANUARY 20TH 2006  
MITS meeting 2006  
International Conference of Materials Databases

ACKNOWLEDGEMENTS
DATA MINING

Original Data

Data Warehousing

Preprocessed Data
(Importing / Combining / Sorting / Linking / Exporting)

Feature Extraction

Transformed Data

Data Mining & Visualization

Knowledge

Patterns

Interpretation

DATA MINING and USER INTERFACE

Database

Repository

Large Scale Multivariate Database

Numerical data

Image data

Computation Interface between Data & User
Transparent Web Based Interactive System

1. Large Scale Multivariate Database

2. Data Warehousing

3. Feature Extraction

4. Data Mining & Visualization

Input: Experimental / Computational Data

User

Output: Structure-Property Relationships

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**DIMENSIONALITY REDUCTION**

*M compounds N descriptors*

- **DATA MATRIX:** latent variables / response metrics

  - Principal component analysis:
  - Goal is to find a projection that captures the largest amount of variation in data

  - Principal component (eigenvector) space:
  - Each PC is described as a linear combination of the weighted contribution of each variable
  - with \( PC_i = \sum_{k} w_{ik} X_k \) where \( w_{ik} \) are weights

  - **Binning / clustering:**
  - Each data point represents a correlation position of compound as influenced by all descriptors

  - Seek patterns of clustering in PCA space which may involve other statistical and data mining techniques: integrate into materials science interpretation for knowledge discovery

**DATA BASE DEVELOPMENT**

- **Topological descriptors**

  - **Framework density (FDSi):** 17.6 T/1000Å³
  - **Ring sizes (# T Atoms):** 8 6 4
  - **Secondary Building Units (SBU):** 8 6 4
  - **Coordinates of T-Atoms in space group Ima**:
    - Site Multipl. x y z
    - Symmetry Restrictions
    - T1 8 0.3427 0.2500 0.4007 X,1/4,Z
  - **Coordination Sequences**
    - Vertex Symbol
    - T1 4 10 21 36 54 78 106 136 173 214
    - Loop configuration of T-atoms: T1

- **Space Group descriptors**
  - **Space group #**
  - **Presence of:**
    - Symmorphic behavior
    - Screw axis
    - Glide plane
  - **Point group**
  - **Lattice type**
  - **Lattice parameters**
  - **Lattice parameter ratios**
    - c/a, b/a ....
    - **Metric tensors**

**KRISHNA RAJAN**
## The enumeration scheme for descriptors

<table>
<thead>
<tr>
<th>ID</th>
<th>Descriptors</th>
<th>ID</th>
<th>Descriptors</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>SBU1 nodes</td>
<td>19</td>
<td>a</td>
</tr>
<tr>
<td>2</td>
<td>SBU1 connections</td>
<td>20</td>
<td>b</td>
</tr>
<tr>
<td>3</td>
<td>SBU1 one-connected nodes</td>
<td>21</td>
<td>c/a</td>
</tr>
<tr>
<td>4</td>
<td>SBU1 two-connected nodes</td>
<td>22</td>
<td>a/c</td>
</tr>
<tr>
<td>5</td>
<td>SBU1 three-connected nodes</td>
<td>23</td>
<td>exp(a/c)</td>
</tr>
<tr>
<td>6</td>
<td>Space group descriptors</td>
<td>24</td>
<td>b/a</td>
</tr>
<tr>
<td>7</td>
<td>Symmorphic or not</td>
<td>25</td>
<td>a/b</td>
</tr>
<tr>
<td>8</td>
<td>Presence of screw axis</td>
<td>26</td>
<td>exp(a/b)</td>
</tr>
<tr>
<td>9</td>
<td>Presence of glide plane</td>
<td>27</td>
<td>b/c</td>
</tr>
<tr>
<td>10</td>
<td>Crystal system</td>
<td>28</td>
<td>γ</td>
</tr>
<tr>
<td>11</td>
<td>Bravais lattice</td>
<td>29</td>
<td>γ/β</td>
</tr>
<tr>
<td>12</td>
<td>P</td>
<td>30</td>
<td>γβ/α²</td>
</tr>
<tr>
<td>13</td>
<td>B</td>
<td>31</td>
<td>exp(γβ/α²)</td>
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<tr>
<td>14</td>
<td>C</td>
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<td>γα/α</td>
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<td>I</td>
<td>33</td>
<td>αα/γ</td>
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<tr>
<td>16</td>
<td>F</td>
<td>34</td>
<td>bβγ</td>
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<tr>
<td>17</td>
<td>R</td>
<td>35</td>
<td>bγ/β</td>
</tr>
<tr>
<td>18</td>
<td>Point group</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**PC scores plot**

- Lattice constants
- Derived descriptions
- Space groups
- SBU information

**PC 1 (22.76%)**

**PC 2 (15.09%)**

**Descriptors:**
- Space group
CLASSIFICATION TRENDS

Asymmetry due to c/a

PREDICTIONS
The five topologies of Wigner–Seitz cells

<table>
<thead>
<tr>
<th>W–S cell topology</th>
<th>Number of faces</th>
<th>Number of vertices</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>14</td>
<td>24</td>
</tr>
<tr>
<td>II</td>
<td>12</td>
<td>18</td>
</tr>
<tr>
<td>III</td>
<td>12</td>
<td>14</td>
</tr>
<tr>
<td>IV</td>
<td>8</td>
<td>12</td>
</tr>
<tr>
<td>V</td>
<td>6</td>
<td>8</td>
</tr>
</tbody>
</table>

The 24 types of Wigner–Seitz cells

<table>
<thead>
<tr>
<th>Topology</th>
<th>Crystal system</th>
<th>I</th>
<th>II</th>
<th>III</th>
<th>IV</th>
<th>V</th>
</tr>
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<tbody>
<tr>
<td>Cubic</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>Tetragonal</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Trigonal</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Orthorhombic</td>
<td>2</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Monoclinic</td>
<td>2</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Triclinic</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Hexagonal</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Symmetry-expanded principal component analysis based on the five intra-annular torsion angles for 500 cyclopentane rings retrieved at random from the CSD. Two degenerate PCs account for >99% of the variance in this dataset and the plot axes are PC1 along x and PC2 along y.
(i) isopointal structures: structures with the same space group and Wyckoff sequence;
(ii) configurational isotypic structures: isopointal structures with similar coordination of the constituents;
(iii) crystal-chemically isotypic structures: configura-tional isotypic structures with similar physical/chemical characteristics of corresponding atoms and bonds.
High speed correlation analysis of large spectral data sets:

- Separation of instrumental and noise effects
- Rapid identification of # of chemical species
- Accentuates signal / noise ratio
- Identify subtle differences in line position and shape effects between spectra
- Model independent method for line shape analysis

Applications to neutron scattering:

- Rapid detection of new phases
- Enhancement of signal/noise helps identify small but real changes in peak shape
- Provides a new tool for rapid calibration of spectra
Multivariate spectral features:
- line intensity
- line breadth
- line position
- instrumental effects

Multivariate materials influences:
- hkl
- phase identification
- influence of cyclic deformation
- defects
- temporal changes in phase stability
- influence of stress state

Ultra large data sets
- Need to detect temporal correlations rapidly yet robustly – detailed Fourier analysis of each peak prohibitive / tracking of very subtle but important changes in spectra
- Materials science issues:
  - Identification of onset of phase changes
  - Influence of stress states over time
  - Role of crystallography of slip and deformation

Time dependent behavior - mechanisms

Spectral Informatics:

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MATHEMATICAL BACKGROUND

$$D_{ixS} = \mu_{ixP} \cdot a_{PxS}$$

$$D = t_1 c_1^T + t_2 c_2^T + \ldots + t_k c_k^T + E = T \cdot C^T + E$$

$$D = \mu \cdot a = T \cdot C^T + E$$

PCA can decompose any set of 'linear' spectra

Principal Components (PCs) give 'pure' spectra for each phase

Amount of each phase proportional to eigenvalues

Position in loads plot gives phase composition of each sample

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"Compression" of over 500 spectra from in-situ neutron diffraction experiments

Each data point in 3d plot below tracks the relative changes in the profile of each reflection for all the 500 spectra simultaneously.
Grains oriented with 220 plane parallel to axial direction preferentially transforming

311 and 200 grains not transforming

PC 3 loading plot from data at state 3 showing HCP phase detects this

Change in area under 200 and 311 peak near zero

Significant decrease to 220 and 111 peaks
DATA INTEGRATION

Phase Field  EBSD/OIM  FEM  Boundary Map

Computer Interface

3D Materials Atlas

TOOL DEVELOPMENT

NRL

1. Large Scale Multivariate Database
   - Repository
     - Numerical data
     - Image data

2. DATA ORGANIZATION

3. FEATURE EXTRACTION / TRACKING

4. DATA MINING AND VISUALIZATION

User

Input: Experimental / Computational Data

Output: Structure-Property Relationships

Transparent Web Based Interactive System ("middle layer")
DATA WAREHOUSING STRATEGY

Large Scale Multivariate Database (images from modeling & experiment)

Data Fusion

Property 1, Property 2, Property 3, Property 4, Property 5, Property 6

X-Y-Z

Data Integration

Property 1

X-Z

~10 million Voxel

N properties and image features……..

GRAIN ID

Distance from a Boundary

DATA WAREHOUSING STRATEGY

Data Integration

Property 1

X-Z

Data Fusion

3D DATA INTEGRATION

FEM

3D Microstructure

3D DATA / MODELING

3D DATA DISCRETIZATION

3D DATA INTEGRATION

σ_{FM|U,\iota}, σ_{FM|V,\iota}, σ_{FM|W,\iota}, τ_{FM|U,\iota}, Grain ID, Distance from a Boundary

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From this step,

1. One attribute (von Mises stress due to x displacement and distance from boundary) in 2D (y=1st plane)
2. Identify spatial points with respect to X- and Z pixels.
3. Not easy to investigate correlations between planes (or properties)
From this step,

1. Two properties ($\sigma_x$ and distance from boundary) in 2D
2. Correlations between properties (+ simple statistics: Regression)
3. Correlations between properties and spatial information (Pixels)
4. Outlier detection
Triple junction - high stress

\[ \sigma_{VM} \bigg|_{U_x} \]

Triple junction – not high stress region for von Mises stress due to displacements in y, z and shear in x-y plane.

**TRACKING TRIPLE JUNCTIONS**

**TRACKING OF CORRELATIONS IN 3D IMAGE**

**Modeling & Imaging**

Data

**Approach**

3D Tracking

Illustrative example:
Identification of 3D Feature (i.e. triple junction) as a stress outlier: “hot spot”

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CONCLUSIONS

- Search and retrieve
- Refining descriptors
- Developing predictions
- Filling in missing data

- Structure databases
- Diffraction spectra databases
- Hyper spectral imaging databases

Mapping / Visualization of databases:
- Correlations
- Trend analysis

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XML-based data management for combinatorial materials science

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Abstract:

Combinatorial synthesis can be used to produce rapidly large numbers of different materials. Different samples are typically organized in sample libraries that can be quickly characterized. Such experiments produce large volumes of characterization data that needs to be stored, processed, shared, and archived. One possible implementation of a web-based data management, storage, and sharing system is described in this presentation. We propose a XML-based data handling system that can be used to manage combinatorial solid state materials science experiments. We also illustrate some of the advantages of a unified data format for data manipulation.
XML-based data management for combinatorial materials science

Mikk Lippmaa
Institute for Solid State Physics
University of Tokyo

S. Meguro
T. Ohnishi
H. Koinuma
and
The Comet Community

I. Takeuchi
University of Maryland

Outline

- What limits efficiency of combi experiments
- Data types
- Library types
- Data representation (XML)
- Data mapping and visualization
- Combining data sets
Combinatorial chemistry

Made famous by massively parallel drug development experiments

For organic synthesis, the keywords are:

- multiwell plates
- carrier / binder / linker
- robotic sample manipulation
- parallel screening
- data processing

Applications of combinatorial techniques

Good examples of high-throughput synthesis

Good examples of high-throughput analysis

What limits experimental productivity?

(data analysis)
Background: materials

perovskite  \( K_2NiF_4 \)  spinel  etc.

All are layered compounds

Explore structural complexity

Explore compositional complexity

Thin film combinatorial design

inorganic thin films  \( \rightarrow \)  organic synthesis

bulk-like materials

non-equilibrium structures

superlattices nanostructures devices
Solid-state thin film synthesis of (mostly) transition-metal oxides

Pulsed Laser Deposition of oxide thin films

Background: properties

Very many different properties are being looked at

properties

dielectric behavior
leak currents
thermopower
band gap control
magnetic ordering
resistivity
superconductivity
ferroelectric behavior
relaxor behavior
luminescence
optical absorption
catalytic activity
etc.

many (more or less)
high-throughput
characterization
techniques

XRD magnetization SQUID-microscopy
AFM optical absorption STM
SEM luminescence RHEED
TEM IR LEED
R-T NMR AES
I-V μ-wave microscopy ICP
C-V CAICISS SR-UPS/XPS
CXRD

Comet
Library types

Several different library types are in use:
- cells
- gradients
- devices
- wells
- capillaries
- etc.

Library data needs to be mapped onto a phase diagram

The role of informatics in materials science

The traditional way

1. Sample design
2. Synthesis
3. Characterization
4. Visualization
5. Analysis

low 'bit rate' process

The combinatorial way

1. Library design
2. Synthesis
3. Characterization
4. Visualization
5. Analysis

A 'broadband' process

The greatest barrier is fast and efficient access to information, which is why visualization and analysis tools are very important.
Data rates

The really high data rates are elsewhere, e.g. CERN Large Hadron Collider, Compact Muon Solenoid

Data produced at up to 1Tbit/s
Real-time processing
Compute farms
Petabyte storage, etc.

Phase space mapping

- Usually composition gradient library
- Limited number of characterization techniques
- May produces large quantities of repetitive data (XRD)
- Visualization and processing issues
- Moderate repetitive raw data volume
  (XRD 10GB/day, Spectroscopy 10MB/sec)
  Requires instrument-specific analysis software
Focused study of a particular material system

- Relatively small number of samples within a certain family of structures, e.g. (TM):TiO₂
- Complicated characterization, many techniques

Small number of samples and relatively low volume of processed data
Many different forms of measurement results need to be combined, reliability and validity of each measurement needs to be evaluated

Problems that we need to solve

Data volume is moderate after initial extraction of data from raw measurements
Data variety is large
Different library types
Mapping of characterization data back to the phase diagram
Present state of materials data availability

- Statistical structure-property analysis benefits from large data sets ($10^4$ - $10^5$ samples)
- Such data sets do not exist. Combinatorial solid-state synthesis can, in principle, start to produce such data sets.
- Current combinatorial libraries contain 10 - 1000 samples
- Existing materials databases have limited usefulness: Only simple compounds, e.g. binaries, are systematically listed. Collections like Landolt-Bornstein are not digitally readable.

- How to build information collections that are statistically useful?

Informatics components

Informatics is a broad term. The following items are included:

- data access
- library design
- instrument control
- instrumentation
- data exchange
- combining data sets
- external data sources
- data storage formats
- electronic notebook
- searching
- visualization
- data publishing
- statistical analysis
- data mining
- analysis
- access controls
- user interface

highest value!
Communications

Current COMET collaboration:

- NIMS (Tsukuba)
- University of Tokyo (Kashiwa and Hongo)
- Tokyo Institute of Technology (Yokohama)
- Tohoku University (Sendai)
- KAST (Kanagawa)
- Photon Factory (Tsukuba)
- Shizuoka University
- University of Maryland (USA)
- etc.

A single library may be processed or analyzed at 2 or 3 different sites.

Communicating data quickly between project members is a priority.

How to reach the highest-value items?
(visualization, statistical analysis, data mining)

Experiments and experimental procedures need to be designed with later analysis in mind:

- Experimental data must be properly documented
  - How was the data obtained
  - What was measured
  - Sample identity and history

- All experimental results need to be stored
  - Sample library processing history
  - All characterization data
    (during screening we may only be looking at a limited subset of data)

- Data storage formats must be standardized, e.g. XML
  - Data exchange between applications
  - Data exchange between research groups
  - Data exchange between databases
XML works as a 'neurotransmitter' between components

The informatics system

Comet

Web browser

LAN or Internet

Web interface

database server

SQL

measurement instruments (hardware tools)

visualization analysis data mining (software tools)
Advantages of a Web-based design

- Web browsers are always available, on many platforms
- Can access experiment data from any source, even from a firewalled environment.
- Access control tools and encrypted communications (SSL) are widely available in Web browsers
- Fast graphical access to experimental data
- A web interface can be used either by human users (using a browser) or by automated tools (web services)

Difficult to build an interactive real-time processing or visualization tool. Can rely on external applications.

Software selection

Operating system: Linux
Storage: 900GB RAID5 array
Backup: 80GB DLT tapes and 300GB removable SCSI disks

Relational database: PostgreSQL

Dynamic Web page generation and web services: PHP scripting language

Web server and access control: Apache

Network access: HTTP over SSL
Allow secure access over public networks
The user interface

Fast access to all information related to a combinatorial library, from design to characterization and analysis.

Currently supports these data types:
- Text
- Images
- PDF files
- AFM images
- XRD data
- etc.
XML: eXtensible Markup Language

- XML is used for formally describing the structure of information, i.e. specifying what each data item means.
- HTML, one dialect of XML is commonly used for creating Web pages.
- Data from an AFM measurement could be represented like this:

```
<afm>
  <sample>TY277</sample>
  <id>37763</id>
  <type>friction</type>
  <area>2E-6</area>
  <lines>256</lines>
  <points>256</points>
  <speed>60</speed>
  <date>21-10-2003</date>
  <data>12777 12792 12922 13144 ...</data>
</afm>
```

This part consists of metadata that gives a description of what was measured and how the measurement was done. This information is useful for organizing, processing and searching of data.

This is the bulk image data that can be used for creating images or for further numerical analysis.

---

Defining the grammar of an XML vocabulary

- A schema definition file defines the logical structure of an XML file.

```
<xsd:schema xmlns:xsd="http://www.w3.org/2001/XMLSchema">
  <xsd:element name="AFM">
    <xsd:complexType>
      <xsd:annotation>
        <xsd:documentation>
          This element defines the content model for AFM (Atomic Force Microscope). It attribute shows measurement data. "Type" element contains Note, MeasurementPoint, MeasurementArea, Setup, OptionalSetup, Data and Images child elements. Note element has comment text entry.
        </xsd:documentation>
      </xsd:annotation>
    </xsd:complexType>
  </xsd:element>
  <xsd:element name="Sample">
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          This element contains the name of the sample.
        </xsd:documentation>
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  </xsd:element>
</xsd:schema>
```

- Independent developers can create software to process the same data.
- Allows automated manipulation of data structures
Examples of public XML schema

PANalytical XRD data format - XRDML
http://www.xrdml.com/

Scanning Probe Microscopy Markup Language - SPML
University of Twente
http://smi.el.utwente.nl/SPML/
http://spml.net/

Chemical Markup Language - CML
http://www.xml-cml.org/

Materials Markup Language - MatML
http://matml.nist.gov/

We have added XML schema for

Microscopy: Atomic force microscopy (AFM), Scanning electron microscopy (SEM)

Various forms of x-ray diffraction: $\Theta/2\Theta$ XRD, concurrent XRD, GADDS (Bruker)

Electron diffraction (RHEED)

Composition analysis (EPMA)

Electronic properties (PPMS)

etc.

Next step: combining data sets

Example: magnetic materials
- library layout
- composition analysis
- magnetic characterization
- structural analysis (XRD)

Library layout
Composition (library map)
Composition (phase space)
Magnetization (library map)

XRD is much harder to visualize

Thanks to XML, the mapping is automatic
Data mapping

The XML data is organized around cell index numbers

We still need instrument-specific mapping of data from raw data to calibrated library coordinates.

Gradient libraries

For gradient libraries we can define a virtual cell mask

Step 1: Transform points from measurement coordinates to physical library coordinates

- rotation
- translation
- nonlinear transforms?

Step 2: Define a virtual library mask, map data to mask

Measurements that fall within a single cell represent the same composition
What next?

Uses for well-organized data in a well-defined format:

Build larger data sets for statistical analysis?

Publishing raw data in addition to results?

Replacing traditional materials databases by intelligent search?

Conclusions

- Combinatorial experiments produce data that is difficult to analyze efficiently without specialized tools

- For us, the main problems are related to the complexity of the data rather than the volume

- We suggest an XML-based data representation

- Using XML as a standardized data storage and exchange language lets us build an informatics system in a heterogeneous environment piece by piece

- XML encoding helps to build generic data processing tools that can be applied to many unrelated data types
Materials portal active in March 2006 at http://e-materials.net/

XML schema definitions & discussion
On-line database software
1. Introduction

One of the most challenging tasks in material science is designing materials with certain atomic constitutions, which achieves some distinct properties. With the spectacular development of information technology and computational techniques, people have been dreaming to design materials with specific properties from all possible atomic combinations by using powerful computational physics. However, the huge amount of possibilities to be treated is still out of the manageable scale. Nowadays, a combination of two types of approach, the data-driven approach based on the comprehensive materials database and the model-driven approach based on the first principles calculation, is proposed as an efficient way to accelerate the speed of finding target atomic configuration from huge number of candidates.

2. Data/Model-driven approach

Mapping approach is utilized by mining the data in materials databases for discovering the regularities and correlations on the compound formation, constitution and crystal structures, which directly provide hints on candidate materials in preliminary stage. The basic idea is to relate a kind of “compound property” to one or several parameters of the constituting elements and to implement “mapping” by taking these elemental parameters as the axes in the discovery space. The aim of mapping is to group data with certain property into clearly defined domains, so as to reveal the patterns of various dependence of the property on the coordinates. There are two key points in mapping: how to select atomic properties as the coordinates of the map and how to define the domains according to the purpose.

On the basis of regularities revealed by data mining, various theoretical approaches are applied to the target substances for investigating further their structural stability, phase equilibrium, and physical properties in order to estimate the possibility to be new materials and to understand the insight into the origin of those regularities.

3. Examples

Two examples are presented to show how this combined approach is attempted towards materials design.

1) Theoretical structure map

Since the materials data available are far from filling the mapping space, there should be some uncertainty in determining the boundary of different mapping domains. The computational data would provide a complement to the experimental data in the mapping space. The systematic calculations on carefully selected physical model will be possible to create a “theoretical structure map”. A preliminary study has been done on $AB$ intermetallic compounds.

2) Discovery of new H-storage substances

Structural mapping is applied to a limit number of well known binary hydrogen storage alloys. Within a large number of combinations of elemental properties, it is found surprisingly that all of these known binary hydrogen storage alloys are allocated in a straight line in the two-dimensional space by taking the average valence electrons number and average electronegativity of these systems as the coordinates. In order to search new hydrogen storage alloys, we plotted all binary systems with 28 most common structure types into the same space as the known binary hydrogen storage alloys, systems at or quiet near the straight line are picked out as the initial candidates. After screening by evaluating the volume of empty space in certain crystal structure, several binary compounds are selected as potential new hydrogen storage substances. The further judgment of the feasibility of formation and the prediction of relevant physical properties are subjected to various theoretical calculations on these binary substances and their hypothetical hydrides.
Outline

I. Introduction: materials design
II. Approach
   - Data-driven approach: data mining
   - Modeling-driven approach: ab initio
   - Data/Modeling-driven approach
III. Examples
   - Structural map:
     empirical, calculated
   - Discovery of new H-storage materials
I. Introduction: Materials Design

Too many Possibilities…?

Design

Periodic Table of the Elements

Materials
Unary
Binary
Ternary
Quaternary...
Multinary

Prediction (Production Line)

Needs
Functions
Properties
Structures
Atomic Constituents

Materials Design (Resolution Line)

- Specification design
- Function design
- Structure design
- Process design

Basic Idea

- Based on the comprehensive materials database to reveal regularities:
  - Formation of compound in a given binary system
  - Composition of stable compounds in “compound formers”
  - Structures of a given compound
  - Properties of a given compound

- Postulation

Elemental Property Parameters (EPPs)
Expression

Property of Materials

II. Approaches: Data-Driven Approach

Tool: Materials Databases
II. Approaches: Data-Driven Approach

Mapping

- Purpose of Mapping
  Proper Elemental Properties as Axes
  ↓
  Substances in same/similar structure/properties → Groups

- Two key points in mapping
  Characterization: To find optimal coordinates
  Classification: To define meaning of domains

II. Approaches: Modeling-Driven Approach

Calculations based on various physical models provide:

- Complement to empirical data;
- Further screening and prediction of hypothesis;
- Understanding of insight into the origin;
- Prediction of materials with required properties.
II. Approaches: Modeling-Driven Approach

Theoretical Approaches

- First Principles Electronic Structures (FLAPW, Wien)
- Car-Parrinello Molecular Dynamics (CPMD, VASP)
- Cluster Expansion Method (CEM)
- Cluster Variation Method (CVM)
- Phase Field Method (PPM)
- Classical Molecular Dynamics (MD)
- ......

II. Approaches: Data/Modeling-Driven Approach

Too many Possibilities…?

Design

Regularities

Model-Driven Approach → Origin

Data-Drive Approach → Discovery
III. Example-1 Structural Map

- Two key points in mapping
  - **Characterization**: To find optimal coordinates
  - **Classification**: To define meaning of domains

- Straitage to Find Regularities

```
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<thead>
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<th>3,000 Conventional Structures Types</th>
<th>~30 Atomic Environment Types</th>
</tr>
</thead>
<tbody>
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<td>?</td>
<td>Distribution, Patterns, ...</td>
</tr>
<tr>
<td>56 Element Property Parameters</td>
<td>2-3 Optimal EPP Expressions</td>
</tr>
</tbody>
</table>
```

Optimal coordinates

- 6 most distinct EPP groups
  - Atomic number
  - Group number
  - Mendeleev number
  - Cohesion energy
  - Electrochemical factor
  - Size

- Operations
  - Sum: $EP(A) + EP(B)$
  - Difference: $|EP(A) - EP(B)|$
  - Product: $EP(A) \times EP(B)$
  - Ratio: $EP(A) / EP(B)$
  - Maximum: $\max(EP(A), EP(B))$
  - Minimum: $\min(EP(A), EP(B))$

- EPP
  - $EP(tot) = EP(A) \text{ op } EP(B)$

Example of EPs
- Atomic number
- Mendeleev Number
  - (D. G. Pettifor, 1983, …)
- Atomic radii
- Melting point
- Electronegativity

Mendeleev Number
New classifications

Atomic Environment Type (AET)

- Concept of AET
  Based on Coordinates Polyhedron
- Rules of Constructing AET
  Maximum-gap Rule
  Maximum-convex-volume Rule
- AET Types of a Structure
  Single, Double, Triple, …

→ Number of structure types decreased remarkably ~150, 31 are popular AET for binaries

CuMg: CsCl-type

8 1st n.n. + 6 2nd n.n.

AET: CN14

P. Villars et al. (1987)

Empirical Structure Map with 3 physical ordinates

Successfully separated ~2,500 intermetallic compounds with single AET

x: difference of Zunger’s radii
y: difference of M-B electronegativity
z: sum of valence electrons number

4 most popular AETs

CN4  CN6  CN12  CN14

P. Villars et al. (1983)
Problem of Empirical Structure Map

- Can not provide insight into the microscopic mechanism
- Limited experimental data leads to uncompleted separation of different domains

Combining Theoretical Modeling: Calculated map

Calculated Structural Map for AET: Model, Method

**Model Systems**

AB intermetallic compound
- \( N_v < 3.5 \), s-s, s-p, p-d
- Martynov-Batsanov’s electronegativity \( \chi \)
  \[ \Delta \chi = \chi_A - \chi_B \]
- Atomic valence electronic energy level \( \{ \varepsilon_i \} \)
  \[ \Delta E = E_A - E_B \]
- Pseudopotential radii’s sum \( R = r_s + r_p \)
  \[ \text{Bond length } d \]

**Calculation Approaches**

- **Tight-binding approach**
  \[ E_{\text{tot}} = E_{\text{bond}} + E_{\text{rep}} \]
  \[ E_{\text{bond}} = \sum_i \varepsilon_i \]
  \[ H = \sum_{ia} \varepsilon_i |i\alpha_i\rangle|\alpha_i\rangle + \sum_{ia} |i\alpha_i\rangle|j\alpha_j\rangle + |j\beta_j\rangle|j\beta_j\rangle \]
  \[ h_{ij} = \frac{\hbar}{md} \]
  \[ E_{\text{rep}} = \frac{1}{2N} \sum_{i,j} \Phi(R) \]
  \[ \Phi_{AA}(R) = \hbar^2(R) \]

**Structural energy difference theorem**

\[ \Delta E_{\text{tot}} = \left( \Delta E_{\text{bond}} \right)_{\Delta E_{\text{rep}} = 0} \]

Y. Chen et al. (1996)
Calculated Structural Map for AET: Results

Investigate Origin of structural preference

Influence of $\Delta E$: large $\Delta E \rightarrow$ small $d \rightarrow$ CN4 and CN6

$\rightarrow$ CN4 requires very large $\Delta E$, no in low $N_v$.

Influence of $\lambda$: higher $\lambda \rightarrow$ higher CN: CN12, CN14
Empirical Structure Map with Mendeleev Number

**MN(A) vs. MN(B) Map for 1:1 Binary Compounds (RT)**

- CN 1-3
- CN 4
- CN 6 (-11)
- CN 12 (-13)
- CN 14(-18)
- Non-former
- Former (no 1:1)

P. Villars, Y. Chen et al. (2004)

Empirical Structure Map with Mendeleev Number

**Comparison of 1:1 and 1:3 for single AET Binaries**

A. Moteki et al. (2003)
AET distribution of Ternary compounds

M. Suzuki et al. (2004)

Challenge: Physical Meaning of AETs

“Structure Group” ↔ “CN Group”

For 5 most popular AETs

CN4: C-like structure
CN6: sc-based structure
CN12b: fcc-based structure
CN12d: hcp-based structure
CN14: bcc-based structure

“CN Group” ↔ “Building Block”: Bonding, Energy, …
III. Example-2: Discovery of New H-Storage Materials

Starting point
32 Already known H-storage alloys (HAS)

Surprising linear relation for known HSAs
Average valence electrons vs.
Average electronegativity

III-2. Discovery of New H-Storage Materials

linear relation for known HSAs → Candidates of new HSAs

Further screening by large unfilled volume
III-2. Discovery of New H-Storage Materials

First Principles Calculation: $A_{n}B_{m}, A_{n}B_{m}H_{q}$

- Possible H sites, structures, stability
-Interstitial volume, Storage capacity
- Electronic structure, binding
- Formation energy, Dissociation pressure

→ Candidates of New H-storage alloys!

IV. Summary

- A combination of two types of approach, the data-driven approach based on the comprehensive materials database and the model-driven approach based on the first principles calculations, provides an efficient way to accelerate the speed of finding target atomic configuration from huge number of candidates.

- Further challenge issues:
  Theoretical investigate - physical meaning of AET, Mendeleev Number, and relevant regularities;
  Application - To various groups of materials with specific properties.
Development of a Materials Risk Information Platform

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1. Introduction

Energy-saving technologies are being developed in various sectors with the aim of reducing environmental loads and using resources more effectively to prevent global warming. This is the case in thermal power generation plants. Power plants that operate at high temperatures are being developed, along with advanced heat-resistant steels to be used in these plants.

The microstructures of heat-resistant steels change during usage, and such changes influence creep deformation behaviors, nucleation and growth of damage, and fracture modes, and consequently creep rupture lives. We therefore need to clarify the main factors influencing microstructural changes, creep deformation properties, nucleation and growth of damage, fracture modes, and rupture lives, and to be able to control these factors. However, because various factors are involved in material properties in a complex fashion, they cannot be determined with good accuracy, and always contain elements of uncertainty. In other words, because the properties of industrial materials have a probabilistic nature, these materials carry the possibility of being unable to fulfill their functions under some circumstances. In addition, we need to evaluate the magnitude of the potential damage caused in the event of failure of these materials. In other words, thinking based on risks is required for optimal selection of materials.

In this report, we describe the necessity of risk-based thinking in the selection of proper heat-resistant steels (and high-Cr heat-resistant steels in particular) and in their proper usage. We also describe the contents and developmental status of the Materials Risk Information Platform that is been has being developed as a database for use in risk assessment.

2. Importance of Accumulation of Long-term Creep Data

In response to demand for boiler operation under high temperatures, heat-resistant steels have been developed and the creep data necessary for designing boilers using these steels have been systematically obtained in the USA, United Kingdom, and Germany. In Japan, creep test facilities have been built at National Institute for Materials Science (NIMS), formerly National Research Institute for Metals (NRIM), to meet strong demand from industry. The Creep Data Sheet Project was initiated in 1966 by setting a target to obtain creep rupture data through more than 100,000 hours of tests of domestically manufactured heat-resistant steels and alloys. The Project is still continuing. Most of the creep data-collecting activities in other countries except Japan are presently suspended. In Europe, a new European Creep Collaborative Committee (ECCC) was established in 1992, and the Committee has been conducting creep data acquisition, collection, and analyses [1].

Development of heat-resistant steels to be used in high-efficiency elevated-temperature power generation plants was started in the 1980s in light of the importance of taking measures to deal with global environmental issues, and these steels have been employed in Ultra Super Critical Boilers. Therefore, acquisition of creep data on advanced heat-resistant steels began at NIMS at the end of the 1980s. Meanwhile, the number of overaged power generation plants has increased in Japan, and more than 80% of the plants have been in operation for over 100,000 hours. Therefore, maintenance and inspection technologies and life evaluation methods must be developed for these plants, and it is important that we develop the ability to predict the remaining lives of materials used in the long term. Consequently, NIMS has been publishing photographic collections of microstructures obtained from the long-term crept specimens.

3. Long-term Creep Properties of Heat-resistant Steels

3.1 Deviation of Creep Strength Data

The main element of steel materials is iron. Various chemical elements are added to the iron to produce various characteristics. Furthermore, various tramp elements are contained in the raw materials and scrap, and these elements are trapped into the steel. Thus, steel materials contain not only the intended alloy elements but also small amounts of unnecessary elements. These unnecessary elements cause deviation in the properties of the steel material.

Fig. 1 shows creep rupture data on 18Cr-8Ni steel (SUS304), a representative heat-resistant steel [2].
This figure gives the creep rupture data of nine heats of this steel. It shows that creep strength varies greatly from heat to heat. The heats with good creep strength contained large amounts of Mo, but one heat had good creep strength even though it contained only small amounts of Mo. One reason for this high creep strength was the presence of large amounts of niobium (Nb + Ta) and moderate amounts of nitrogen (N) [3]. The relationship between the stress and rupture life of each heat showed that the deviation of creep strength for one heat was small. In light of this fact, it is important in using heat-resistant steels that we understand the effects of the chemical elements and production processes, such as heat treatment, that affect creep strength properties, and make use of these effects.

3.2 Microstructural Change during Service and Creep Life

When heat-resistant steel is used in a high-temperature environment, the microstructure of the steel changes. As a result, the creep strength properties also change. Because the original creep strength properties become poorer, this phenomenon is called the deterioration of characteristics. Fig. 2 compares observation data on the creep rupture strength of 1Cr-0.5Mo steel and a curve predicted from the values obtained by analyzing the creep strain curve [4]. The creep strain curve of this steel has two minimal values of creep rate. For this reason, the analysis was conducted by separating the creep strain rate curve into two regions, before and after the creep strain curve. We found that the creep deformation characteristics were affected by changes in the metallic microstructure of the steel and that this change strongly affected the rupture life.

The creep strength of Mod. 9 Cr-1 Mo steel rapidly decreases beyond 10,000 hours at 600 °C; therefore, the creep strengths predicted from short-term creep data are dangerously high [5]. Recovery of the tempered martensitic microstructure of Mod. 9Cr-1Mo steel progresses rather uniformly in the high-stress and short-term creep region. However, in the low-stress and long-term creep region, recovery is uneven because it progresses preferentially near the prior γ-grain boundary. Fig. 3 schematically shows the stress dependency of the microstructural changes in the steel during recovery and the effects of changes in stress dependency on creep strength [6]. The microstructural change of the steel in response to uneven recovery seems to accelerate the reduction in creep strength. For this reason, it is not desirable to predict creep life using high-stress data. Kimura et al. proposed a method of predicting creep life by using creep rupture data obtained in response to stresses that were less than half of the 0.2% yield strength [5]. The predicted curve agreed well with the observed data.

4. Shift from Reliability Engineering to Risk-based Engineering

The strength of heat-resistant steels in practical use varies from heat to heat with the effects of the production procedures; for example, apart from the set chemical composition there may be small amounts of tramp elements, or differences in the processing conditions. The strength of steels also decreases with changes in microstructure during service. The extent of this decrease is affected by the chemical elements present. As mentioned above, the predicted value of creep life varies with the selected prediction method. For this reason, it is necessary to handle the characteristics of the steel material statistically. Fig. 4 schematically shows deviations in material properties and predicted values. On the other hand, the temperatures and loads to be added to the materials also fluctuate. Thus, even if a sufficient safety allowance is secured in the initial period, the statistical distributions of the material-strength properties and external forces unfortunately overlap with each other, and there is a possibility of creep failure. It is the role of reliability engineering to consider the possibilities and probabilities of failure.

As a result of analysis and inspection, however, if there are two structural components that indicate the same failure probability, the problem then lies in deciding which takes priority for replacement or repair. One guideline that may help give a solution is risk management. The risk is evaluated as a combination of the probability of occurrence of failure and the degree of damage that would be caused by the failure:

\[ \text{Risk} = \text{Likelihood} \times \text{Severity of consequence} \]

In risk management, the potential hazard (danger) to be inflicted on people, property, society, and the environment is clarified and the probability of failure is analyzed. The degree of damage is calculated on the basis of past experience, and the risk is assessed. In an actual case, the degree of damage is often calculated by the monetary cost of the damage.

In a risk assessment, the structural component in the plant to be assessed is selected and the condition of breakage or damage to the component is estimated. Then, the probability of failure corresponding to the damage mode of the component is calculated and the amount of damage is also estimated. As shown in Fig. 5, a risk matrix is prepared by the risk assessment method and the acceptability of the assessed risk is evaluated. This method of using a risk matrix is qualitative but simple. If the assessed risk is not acceptable, a measure to reduce the risk is considered and the risk is reassessed. By repeating this risk assessment until
an acceptable risk level is reached, the measures necessary to reduce the risk are taken.

To establish risk-based engineering from a materials engineering viewpoint, it is necessary to (1) clarify the uncertainties of material properties, (2) improve the accuracy of life prediction, (3) improve the accuracy of strength analyses of structural components, and (4) improve the technologies used to detect material deterioration and damage. Further, it is necessary to accumulate knowledge related to, and basic data to support, risk-based engineering.

5. Development of a Materials Risk Information Platform

As described above, there was a need to provide the data and information required for risk assessment in the materials engineering field. For this purpose, research and development of a Materials Risk Information Platform to improve data and information for risk assessment and support risk assessment were commenced in 2001 by NIMS (the Platform’s central core), as well as by other participants, such as private research organizations, universities, and related associations and societies [7]. As it is relatively easy to collect the necessary data and information and a certain amount of know-how had been accumulated for this project, the boilers of thermal power generation plants were selected as research subjects, and the research began. The research themes are the determination of factors affecting the lives of materials and components; improvement of the accuracy of life prediction; collection of information related to microstructural change; preparation of photographs related to microstructures; development of equipment diagnostic support systems (such as the tools needed for strength analyses of structural members); preparation of a database of accident cases; and preparation of an allowable stress database. The results of these studies will be finally put together into the main system of the Materials Risk Information Platform, as shown in Fig. 6. Various other databases (such as NIMS’s Structural Materials Database) that are needed for risk assessment will be linked to the Platform. The Materials Risk Information Platform will open to the public through the Internet in April 2006.

6. Sharing of Materials Information

Material properties are complex because of the influences of various factors. Therefore, the content of a database that specializes in materials needed to be based on profound knowledge. However, the capacity of the database would be limited, and a single database could not cover all of this wide field. Therefore, if we were to obtain accurate solutions by using the materials database, the database needed to be versatile. NIMS liaised with the Material Data Network developed by Granta Design Ltd., represented by Prof. Ashby of the University of Cambridge, and facilitated the retrieval of necessary information by users [8]. This Material Data Network is linked with U.K. and U.S. materials databases, and users can locate information they want to obtain among such linked databases. The numbers of data hits obtained when “creep” and “2.25 Cr-1 Mo steel” are input into the system are shown in Table 1. The table demonstrates the abundance of creep information, but when “2.25 Cr-1 Mo steel” is input, not only the number of data hits drops, but also some strange numbers show up. For example, the number of data hits retrieved from MatWeb increases, but these data are not retrieved from the NIMS materials database. This indicates that, although voluminous amounts of data on 2.25 Cr-1 Mo steels are contained within the NIMS creep database, these data were not retrieved: further improvement is required because the system is not perfect. In the process of risk assessment, not only the assessment process but also the data and information used need to be transparent. In addition, these data must be transparent to everybody.

In other words, as risk-based engineering of materials becomes used increasingly, the importance of making such information publicly available will continue to increase. Moreover, because data and information must be impartial, the role of the NIMS database, prepared at the discretion of NIMS, will be considered ever more important as the Institute continues to obtain standard and reference data and make them available to the public.

7. Conclusions

Our society needs to be safe and secure, but we also need to accept a certain level of risk if we are to reap the benefits of research in the sciences and technologies. In risk-oriented societies, the development of materials and studies of material reliabilities should be conducted in accordance with risk-based engineering. This paper has dealt with high Cr heat-resistant steels; it describes the importance of adopting risk-based concepts in the use of heat-resistant steels by clarifying their creep strength properties and fully utilizing their characteristics. The method of development of risk-based engineering is not much different from conventional development methods. The important points are to further redevelop subjects that have already been developed and to accumulate information on their use (including accident cases); to recognize
certainties and uncertainties; to develop safety analysis technologies by taking into account quantitative concepts; and to open these basic data and information to the public so that users can easily judge them.

References


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<th>120</th>
<th>140</th>
<th>160</th>
<th>180</th>
<th>200</th>
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<td>Time to rupture (h)</td>
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<td>10^2</td>
<td>10^3</td>
<td>10^4</td>
<td>10^5</td>
<td></td>
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</table>

![Fig. 1. Creep rupture strength of 18Cr-8Ni steel (SUS304)](2)
**Fig. 2.** Calculated creep rupture life of 1Cr-0.5Mo steel [4]

**Fig. 3.** Schematic illustration of stress dependence of microstructural change during creep exposure at elevated temperatures and its effect on creep strength [6]
**Fig. 4** Schematic illustration of probabilistic failure of materials during creep

**Fig. 5.** The risk matrix: sample result from the Materials Risk Information Platform
Fig. 6 Structure of the Materials Risk Information Platform

Table 1. Numbers of data hits obtained from a Material Data Network search

<table>
<thead>
<tr>
<th>Input word</th>
<th>ASM Handbook</th>
<th>ASM Alloy Center</th>
<th>ASM Micrograph</th>
<th>ASM Failure Analysis Center</th>
<th>MatWeb</th>
<th>MIL-HDBK-5H</th>
<th>NIMS Materials Database</th>
<th>NPL MEDAS</th>
<th>The PGM Database</th>
<th>SteelSp ec II</th>
<th>TWI JoinIT</th>
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<td>318</td>
<td>2</td>
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<td>55</td>
<td></td>
<td>8</td>
<td>426</td>
<td>5259</td>
</tr>
<tr>
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<td>17</td>
<td>—</td>
<td>9</td>
<td>5009</td>
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Introduction of KISTI’s Factual Databases

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1. Introduction

Generally, the factual database seems to be very difficult to develop because it takes a lot of time and budget to build up. Moreover, the contents of factual database is focused on a special subject in science and technology, the range of user is limited to a certain subject and the number of users is not so increased as it is like a bibliographic information. In addition, as the scientists who develop a certain factual database would finish their project, the fund that support the factual database is stopped and the factual database is not updated any more. So the factual database that could update its contents regularly is rare seen in Korea.

Around 2000, KISTI are interested in developing the factual database in Korea, and investigate some factual databases that seemed to be very useful in academic and industrial field. KISTI selected some of factual database to build up and they are supported by the fund given by Korean Government.

In this paper, we will introduce some KISTI's factual databases. These databases are now yearly updating by corresponding institute or university and you can obtain the more detailed information by visiting the corresponding web site.

2. Several KISTI's Factual Databases

2-1. Chem DB

From 2000, KISTI begin to develop the Chem DB with Bioinformatics & Molecular Design Research Center (BMD). The BMD is a research center that is specialized in designing the new drugs or materials by using the chemoinformatics technology. To support the scientists who are studying in new drug design, KISTI and BMD cooperate to construct the Chem DB that have very useful information for drug design.

In Chem DB, there are about 2 million substances that have 2-D, 3-D molecular structure and their properties. The text(name, CAS-RN and formula) and structure search (exact, substructure and similarity engine) are available and you can obtain the general common information, calculated physicochemical, ADME, drug-likeness properties and their 3D conformers about the specified substance that you search for.

In structure search, You can use the several filter option such as topology, drug-likeness, ADME and reactive group to obtain list of drugable compounds. The web site of Chem DB is http://chemdb.kisti.re.kr/main/main.

2-2. Plasma Property DB

In 2002, Nuclear Fusion Research Center(NFRC) in Korea suggested the proposal of developing the plasma property DB. The proposal is based on the increase of requesting the plasma property data from the small and medium Korean company. In Korea, there are about 300 small and medium scale companies that make the semi conductor manufacturing equipments. The plasma process is related directly or indirectly to over than 80% of the semi conductor process and the position of semi conductor manufacturing industry is very high in Korea. KISTI and NFRC decided to develop the plasma property DB in 2002 and it is now on going.

At present, the plasma property DB has the data of oxygen, hydrogen, nitrogen molecules and also argon and xenon atoms. Also in this year (2005), we provided C4F6 and C4F8 gas data to SAMSUNG. Each atom and molecule database included the structure, spectrum, cross section, and reference data. In the cross section data, according to the incident particle, we divided in 3 kinds, namely, electron collision, heavy particle collision and photon collision. Each particle also has 6 kinds of cross section and these are elastic, ionization, excitation, recombination, detachment and attachment scattering. You can see each cross section of specified particle in graphic figure or numeric data. These data are also linked to the bibliographic reference data source that these data are extracted from.

The plasma property DB is yearly updated. The entering energy standardized with 10 eV and the wavelength was classified according to the molecular state. The data related to the structure was also classified by the molecular state. The data formed in this way are almost 10,000 cases. The web site of Plasma Property DB is http://fact.kisti.re.kr/factdb/pla_infor.jsp.
2-3. Digital Korean DB

The data from the human body are very useful. Many research fields such as medical surgery, industrial safety, biomechanics etc. need the information of human body. In Korea, the information about Korean human body was insufficient and some of them were scattered. So we made the new database of Korean human body. The method for providing information of human body is the construction of human body model. Human body model means the virtual human in computer cyber space. The human model can be used for various experiments instead of real human. This human model was constituted three information about shape, property and movement. From 2003, KISTI and Catholic University Medical College have begun to construct the database of human model. The 1\textsuperscript{st} year(2003) of the project, we made the averaged skeletal model. The skeletal model was made by segmentation area based on CT images (Female: 50, Male: 50 cadavers, 1mm thickness scanning of whole body). The averaged skeletal model was made by our new technique. We used mass center and principal direction of 3-dimensional bone shape to make the averaged skeletal model. In 2\textsuperscript{nd} year(2004), we made the fine skeletal model for hands, foots and teeth that made by segmentation area based on micro CT images. And we also made three kinds of skin model(overweight, normal weight, less weight sample). In 3\textsuperscript{rd} year(2005), we constructed the database for mechanical properties of bone like as elastic modulus, yield strength and ultimate strength. The tests were performed at cortical and trabecula region of bone. We used the indentation test for cortical bone and used the compressive test for trabecula bone. The mechanical properties of bone are essential data for physical simulation such as stress analysis, structure stability and biomechanics.

3. Future Plan

3-1. Chem DB

As the users would like to analyze drug database according to drug activity class and apply analysis results to chemical library, we will divide ChemDB data into 5 parts such as NCI, drug, PhyChem building block and chemical library. Also the substance of natural products will be added its molecular structure.

New pharmacophore search engine to identify the lead structures will be added. The concept of pharmacophore mapping strives to discover the common three-dimensional patterns present in database molecules that act at the same enzyme or receptor target site. Sequentially, 3D filtering method among these substances for pharmacophore search will also be suggested by BMD.

The general information of the substance is not sufficient yet, we will fulfill the more general information such as CAS registry number etc. All the substances in Chem DB have their own mole files, the NMR spectra of each substance could be predicted by NMR predicting software program.

3-2. Plasma property DB

In the plasma DB, cross section data of other molecules will be added in the future. On the technical aspect, the industrial application plasma requires not only the high priced equipment but also advanced control technique, which satisfies the particular conditions required by the industry. Therefore, the data for the basic design and operation/control techniques also will be included in the database.

As one of the most effective methods, the result of the numerical simulation is commonly referred to the basic design before manufacturing the equipment. Thus, the simulation codes that is developed between the scientists will be also registered in the database. In the case of simulation code, which can be accessed by the internet web page, the feedback system could built through opening the source code to the public so that it is complimented to more advanced from between users and by being offered to other users through the program upgrade.

Lastly, the usefulness of the database will be improved by building the system, wherein users exchange the information they need, the manager for database grasps the information, which users need in short time and offer it by forming the open community for the discussion.

3-3. Digital Korean DB

Digital Korean human model is continuously improving from skeletal model to whole body human model. Already, we made the averaged Korean skeletal model and the mechanical properties of bone. Next year we will construct database for muscles, ligaments and internal organs. In the future, when the database is constructed completely, we think Digital Korean Model will be physically almost same to real human. Additionally we will make the model such as circulatory tube, airway, urinary tube model for the research of hemodynamics and computational fluid dynamics.
Introduction of Factual Databases in KISTI (Korea)

Jan. 18-20, 2006
Sang-Ho LEE (shlee@kisti.re.kr)
Korea Institute of Science and Technology Information (KISTI)

ChemDB System  http://chemdb.kisti.re.kr/main/main

Update of chemical DB
Drug-likeness results
ADME results
Physicochemical properties
Web interface

Exact search & Substructure search
Similarity search
Pharmacophore search
Link to other chemical databases

NCBI, Chemfinder, NIST spectroscopy, toxicity, referenced, physicochemical properties
Chemical Data included in ChemDB - I

  - The Open database of the National Cancer Institute
  - This database includes:
    - 250,251 2D structures
    - Human Tumor Cell Line Screening data (logGI50, logLC50, logTGI)
    - AIDS Antiviral Screening data (EC50, IC50, conclusion).

- Drug Data
  - Drugs included in USP Dictionary of USAN (United States Adopted Names) and International Drug Names
  - This database includes:
    - 2,506 2D structures
    - ATC code and Classification code
    - Various physicochemical properties

- PhysChem Data
  - The physical properties database (PhysProp) of Syracuse Research Corporation (SRC) and data of various reagent catalogs
  - This database includes:
    - 41,253 2D structures
    - Physicochemical properties
      - Boiling point, Melting point, density, refractivity, LD50, solubility, pKa, logP, water solubility, vapor pressure, Henry's law constant

Databases included in ChemDB - II

- Chemical Libraries from various suppliers
  - Chemical libraries for Combi. Chem. and HTS of various suppliers
  - Suppliers
    - ASINEX, ChemStar, Maybridge, Chembridge, IBS, and SPECS
  - This database includes:
    - Over 1,500,000 2D structures
    - Supplier information (homepage, e-mail, tel, fax, and address)

- Building Blocks
  - Building Blocks for Combi. Chem. of various suppliers
  - Suppliers
    - Sigma, SPECS, Timtec, Toslab, Otava, Maybaridge, IBS, Enamine, ChemT&I, Asinex, etc.
  - This database includes:
    - 2D structures of building blocks
    - Functional groups
    - Supplier information (homepage, e-mail, tel, fax, and address)
Available information in ChemDB - I

- **2D & 3D chemical structures**
  - Over 2,000,000 2D Chemical Structures
  - 3D Conformers of about 400,000 molecules

- **Chemical information**
  - General information of compounds
    - Common name, IUPAC name, molecular weight, molecular formula, CAS number
  - Experimental physicochemical Properties
    - Melting point, boiling point, logP, Refractivity, water solubility

- **2D descriptors**
  - Calculated physicochemical properties
    - Melting point, Boiling point, logP, Refractivity, Solvation free energy, polarizablity by CDEAP method, Vapor pressure, pKa value by Pallas program
  - Geometrical & topological descriptors
Available information in ChemDB - II

- Drug-likeness and ADME prediction data
  - Drug-likeness prediction result
    - Lipinski’s rule, Lead-like rules, Drug DB-like rules (CMC & MDDR)
    - No. reactive functional groups
  - Predicted ADME properties
    - BBB (Blood-Brain Barrier penetration value)
    - HIA (Human Intestinal Absorption value)

- 3D descriptors
  - 3D geometrical descriptors
    - Van der Waals surface area & van der Waals volume, solvent accessible surface & solvent accessible volume, principal moments of inertia
  - Quantumchemical descriptors
    - dipole moment & its components, HOMO & LUMO energy

ChemDB Search System - Basic Search

- Text search
  - By name, CAS Registry number, Formula
- Exact structure search
- Substructure search
- Similarity search
  - By chi1 & chi3 (path) indices
  - By kappa1, kappa2 & kappa3 indices
ChemDB Search System - Pharmacophore Search

- Pharmacophore

X-ray structure

Active compounds

Various Filters for drug-like library design

- Drug-likeness Filter
  - Lipinski’s rule
  - Lead-like rule
  - MDDR-like rule
  - CMC-like rule

- Reactive functional group Filter

- Absorption Filter
  - Water Solubility
  - HIA (% Human Intestinal Absorption)
  - BBB (Blood-Brain Barrier Penetration)
Plasma Process in Semiconductor Industry

- The cost of plasma equipments occupies up to 40% in the total equipment costs: ~ $8 billion in 2005

Plasma technology issues
- Precise process control for nano device manufacturing
- Trend that the process leads equipment development
- Increase of time and cost for nano process set-up (~73nm in 2005)
- Understanding of surface reaction and plasma phenomena for nano process development becomes increasingly important in both equipment maker and device maker.
NRC Panel on Database Needs for Modeling and Simulation Plasma Processing


Assess the status of current database for modeling, simulation and diagnostics of plasma materials processing.

Make recommendations for strategies to meet cited needs.

Greater and more systematic efforts should be made by Federal and industrial agencies to address database needs with emphasis on plasma surface interactions.

Target chemistries should have a high priority in database development because the applications are currently important and will continue to be important over the next 5-10 years.

What we need → Atomic & Molecular Database

- Gas decomposition path (ex: C2F4→CF2→CF→F)
- Electron impact collision cross-section
  - Electron-Neutral: e+CF4 → CF3+,CF2,F,…
  - Electron-Ion: e+ CF2+ → CF+F
    - Electron beam measurement
    - Quantum theoretical calculations
    - Electron swarm experiment
- Heavy particle reaction rate coefficient
  - Neutral-Neutral , Neutral-Ion , Ion-Ion
- Swarm parameters
  - Drift Velocity, Diffusion Coefficient, Ionization coefficient, …
- Surface reaction
- ……….
**Integrated Plasma Database**

- Electron Impact
- Ion Impact
- Reaction Rate Coefficient
- Heavy Particle Collision
- Simulation Software
- Visualization
- Documentation

**Provide advantages in time to device maker and assist in USER (industry, Institute, University)**

**Integrated Device Manufacturer**

**Integrated Plasma Database**

**DB Structure**

- A, M
- Structure
- Spectroscopy
- Vis. & UV.
- Infra-red
- Microwave
- Etc.
- Collision data
- Electron collisions
- Heavy-Particle collisions
- Photon collision
  - Elastic scattering
  - Ionization
    - cross section
    - Rate coefficient
  - Excitation
  - Recombination
  - Detachment
  - Attachment
Fig. EII_1. Ionization cross section for electron collision with O₂

Fig. EII_2. Ionization cross section for electron collision with N₂
### Reference

<table>
<thead>
<tr>
<th>Reference Number</th>
<th>Author(s)</th>
<th>Title and Details</th>
</tr>
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<tr>
<td>EII_OM_N02</td>
<td>A.V. PHEPLS</td>
<td>JILA Information center report No28, 1978</td>
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<td>EII_XeA_N02</td>
<td>A.V. PHEPLS</td>
<td>JILA Information center report</td>
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<td>A.V. PHEPLS</td>
<td>JILA Information center report</td>
</tr>
<tr>
<td>EII_ArA_E01</td>
<td>F. J. de Heer et al</td>
<td>J. Phys. B Vol 12, 979, 1979</td>
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</table>

### Current Status

<table>
<thead>
<tr>
<th>Current status</th>
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<tbody>
<tr>
<td>Atomic &amp; Molecular Data</td>
</tr>
<tr>
<td>- O₂, N₂, H₂, CH₄, H₂O ... etc</td>
</tr>
<tr>
<td>- Ar, C, Xe, He ...</td>
</tr>
<tr>
<td>- C₄F₆, C₄F₈</td>
</tr>
<tr>
<td>- Gas Chemistry data: SF₆/Cl₂/He, SF₆/HCl/He, SF₆/O₂/He, SF₆/N₂/He</td>
</tr>
<tr>
<td>Simulation code</td>
</tr>
<tr>
<td>- Collisional Radiative code (H, H₂, He, Ar)</td>
</tr>
<tr>
<td>- Neutral transport code</td>
</tr>
<tr>
<td>- chamber design code</td>
</tr>
<tr>
<td>- atomic collision code</td>
</tr>
<tr>
<td>- spectroscopy data analysis code</td>
</tr>
<tr>
<td>Reference</td>
</tr>
<tr>
<td>- NIST, IPP, NIFS ... and other technical reports</td>
</tr>
</tbody>
</table>

- Construction of Database for Human Body
- Construction of 3 Dimensional Physical Human Body Model Database Using Computer Tomography: Geometric Database of Skeletal System
- Geometric Averaging Technique for Individual bones of Human: Using Mass Center and Principal Direction
- Construction of Mechanical Properties Database of Skeletal System
Construction of 3 Dimensional Physical Human Body Model Database Using Computer Tomography: Geometric Database of Skeletal System

<Overall Process>

CT Scanning

Segmentation of bone

Generating 3D skeletal models

Geometric database of skeletal system

CT Scanning

- 57 Male and 50 female cadavers

<table>
<thead>
<tr>
<th>Sex</th>
<th>Number</th>
<th>Average age (years)</th>
<th>Average height (cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Male</td>
<td>57</td>
<td>50.7</td>
<td>165.96</td>
</tr>
<tr>
<td>Female</td>
<td>50</td>
<td>53.9</td>
<td>156.22</td>
</tr>
</tbody>
</table>

- CT scan (1mm slice distance)
- Obtain the image data as DICOM and convert the file to Bitmap format
Segmentation of Bone

- Using segmentation and 3D reconstruction program (Bionix®, version 3.0, Korea)
- Selecting bone area on each CT images by threshold masking and manual masking

CT Image  
Segmentation

Segmentation of bone using Bionix version 3.0

Threshold masking  
Manual masking

Masking in sagittal view  
Masking in coronal view
Generating 3D Skeletal Models

- After generating 3D model, surface smoothening step was done

Contents of 3D physical human bone model DB

<table>
<thead>
<tr>
<th>Contents</th>
<th>File format</th>
<th>DB amounts</th>
<th>Sample number</th>
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<tr>
<td>CT images</td>
<td>DICOM</td>
<td>191,660</td>
<td>male 57, female 50</td>
</tr>
<tr>
<td></td>
<td>Bitmap</td>
<td>191,660</td>
<td></td>
</tr>
<tr>
<td>3D physical human bone</td>
<td>Finite</td>
<td>20600</td>
<td>206 bones x (male 50</td>
</tr>
<tr>
<td>models</td>
<td>element</td>
<td></td>
<td>+ female 50)</td>
</tr>
<tr>
<td></td>
<td>model (for</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>NASTRAN)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
<Purpose>
Many authors issued the feature-preserving averaging technique according to positioning and scaling process using the landmarks, which represent the geometric characteristics of three dimensional surface models. Such a technique should be done by manual procedure, choosing and marking the landmarks on each bone surface before averaging process.

Average 3D anatomical skull (Case Western Reserve University Imaging Lab, USA)

Applying engineering mechanics, we produced another averaging technique without having to use such manual procedure, and made averaging models.
Materials and Methods

- 100 3D skeletal models (male:50, female: 50)

Step 1: Aligning
- We calculated mass center and principal axis of inertia from each models.
- These models were transformed to coincide mass center and to align principal axis.

Materials and Methods

Step 2: Scaling
- Bone models were scaled according to average length data of sampling bone models on z-axis.
Materials and Methods

Step 3: Generating averaged volume
- After establishing voxellar hexahedron space which contain all sampling bone models, we counted the number of overlapping voxels.
- We generated the average of three dimensional surface by displaying all voxels corresponding to the area of normal distribution curve lying above the value subtracting the standard deviation from the average of overlapping number.

```
Count overlap number each voxel
(Example)
...............  
Voxel[n-1]=6, Voxel[n]=8
```

Averaging program
- All steps are processed automatically by this application.

1. Loading Surface file : BNS
2. Loaded Components
3. Graphic window
4. Align Step : Mass center, Direction
5. Manual Align : Align arbitrary angle
6. Scaling : Geo. center, Scaling
7. Voxel Overlap counting
8. Generation Average volume
9. Average Component
Construction of Mechanical Properties Database of Skeletal System

Purpose
- Something to reflect mechanical competence of bone
  - morphological and histological aspect of bone, mechanical properties of bone

- Hierarchical approach to exploring bone mechanical properties
  - whole bone level, tissue level, lamellar level, ultrastructural level

- In this study, tissue level
  - cortical bone <- indentation test
  - trabecular bone <- compression test

- Construction of DB and development of DB access program
Materials and Methods

<table>
<thead>
<tr>
<th>Cadaver number</th>
<th>Sex</th>
<th>Age</th>
<th>Height</th>
<th>Cause of death</th>
</tr>
</thead>
<tbody>
<tr>
<td>05-56</td>
<td>Male</td>
<td>34</td>
<td>190cm</td>
<td>Brain edema</td>
</tr>
<tr>
<td>04-40</td>
<td>Male</td>
<td>70</td>
<td>174cm</td>
<td>Stomach CA</td>
</tr>
<tr>
<td>05-19</td>
<td>Female</td>
<td>48</td>
<td>165cm</td>
<td>Lung CA</td>
</tr>
<tr>
<td>05-32</td>
<td>Female</td>
<td>75</td>
<td>155cm</td>
<td>Natural death</td>
</tr>
</tbody>
</table>

- Test area and specimens

- Extraction of bones from cadaver
- Removal of another tissues except for bone
- Cutting test area for indentation experiment
- Making the specimen for compression test
Materials and Methods

- Indentation test: modulus of elasticity, tensile strength (cortical bone)

- Indenter
Materials and Methods

- Fix table for material (bone)

- Test of indentation
Materials and Methods

- Compression test: modulus of elasticity, yield strength, ultimate strength (trabecular bone)

- Micro CT scanning to display the specimens in DB access program:
  18 µm scanning resolution
Thank you!!
A Computer Matching Technique for Steel Grades Comparison between Different Standards

Hang SU1, Wei Han1, Misako Uchida2, Shigemitsu Kihara3, Xiaoling Chen1, Yongquan Zhang1
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2) Ishikawajima-Harima Heavy Industries Co., Ltd, Tokyo, Japan
3) Best Material Co., Ltd., Tokyo, Japan
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1. Introduction

At the age of global economic integration, a comparative information system of world material standards is very important for material procurement for manufactory industry. Global sourcing requires not only databases for various material standards, but also needs technique to process the material comparing and matching between standard from different countries.

Recently years, artificial intelligence techniques such as pattern recognition and artificial neural networks were applied in data mining and knowledge discovery in database and proofed effectively. In this paper, a computer matching technique named DMS (Data Matching Subsystem) has been put forward for steel grades auto comparison between different standards. By this technique, the basic information of a steel grade, such as compositions, properties, applications, shapes, special properties and delivery states, have been summarized as several mathematic features. With these features, we can calculate similarity degree between different steels, based what the auto matching and auto comparing for steel grade from different standard can be actualize. This technique is applying and evaluating in the development of China-Japan steel grades comparison database co-worked by CISRI, IHI, AT&M and BM.

2. Principle and Method

DMS is designed to actualize data matching automatically between two or more material correlated database system. Figure 1 shows the planning application of DMS in steel grade matching between different standard. The key frame of a typical DMS can be briefed into three parts: Matching Data Set, Similarity Degree Function, and Knowledge Base.

2.1 Matching Data Set

Matching data set defines a standardized data set that abstract the main composition, mechanical properties and other primary features (keywords) of a material. There are different matching data sets for different materials. For alloyed steel database, the matching data set can be summarized as a composition-property matrix and a keywords matrix.
\[
X_{n,N} = \begin{bmatrix}
X_{11} & X_{12} & \ldots & X_{1N} & P_{11} & P_{12} & \ldots & P_{1M} \\
X_{21} & X_{22} & \ldots & X_{2N} & P_{21} & P_{22} & \ldots & P_{2M} \\
M & M & \ldots & M & M & M & \ldots & M
\end{bmatrix}
\] (1)

In which \( n \) represents the total number of steels in database; \( N \) represents the number of element and \( M \) represents the number of property indexes.

\[
K_{n\times4} = \begin{bmatrix}
k_{1}^{\text{shape}} & k_{1}^{\text{app}} & k_{1}^{\text{sapp}} & k_{1}^{\text{deliv}} \\
k_{2}^{\text{shape}} & k_{2}^{\text{app}} & k_{2}^{\text{sapp}} & k_{2}^{\text{deliv}} \\
M & M & M & M
\end{bmatrix}
\] (2)

In which \( n \) represents the total number of steels in database; \( k_{\text{shape}} \) is the shape keywords, \( k_{\text{app}} \) is the application keywords, \( k_{\text{sapp}} \) \( j \) is the specious application keywords and \( k_{\text{deliv}} \) is the delivery state keywords.

### 2.2 Similarity Degree Function

Similarity degree function defines the algorithms to calculate similarity degree between two matching data set. The original consideration of similarity degree function deduced from radar graph (Figure 2)

![Figure 2 The principle of calculate DSC base on radar graph](image)

In which
- \( S_A \) — The area of steel \( A \)
- \( S_i \) — The area of steel \( i \)
- \( S_{Ai} \) — The area of steel \( A \) overlapped with steel \( i \)

Then the composition similarity degree between steel \( A \) and \( I \) can be defined as

\[
DSC_i = \frac{2S_{Ai}}{S_A + S_i}
\] (3)

The similarity degree of properties (DSP) can be calculated in a similar way.

### 2.3 Knowledge Base

Knowledge base contains a series rules about composition and property of materials that have been summarized based on specialist knowledge. These rules were defined to deal with qualitative knowledge that included in material standard, such as “≤”, “≥”, data range, residual elements, micro-alloyed elements, default elements and default properties. For example:

**Data Range Appointment:** When the value of an element or a property (marked as \( X \)) has been given as \( a \sim b \), then appointment typical value of \( X \) as follows:

\[
X = \frac{(a + b)}{2}
\]
3. Development and application

Based on the above matching data set, similarity degree functions and knowledge base, original program has been developed to actualize the material matching between the GB and JIS database. Table 1 shows the comparison of handbook result and DMS matching result between several JIS steel and GB steel. The DMS gives not only correct result, but also gives more detail information than handbook data.

<table>
<thead>
<tr>
<th>JIS steel</th>
<th>Matched GB steel</th>
<th>Handbook result</th>
<th>DMS result (DS ≥ 0.85)</th>
<th>DS = SQRT(DSC × DSP)</th>
<th>DSC</th>
<th>DSP</th>
</tr>
</thead>
<tbody>
<tr>
<td>SS330(SS34)</td>
<td>Q195</td>
<td>Q215A</td>
<td>0.922</td>
<td>0.859</td>
<td>0.989</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Q215A</td>
<td>Q215B</td>
<td>0.889</td>
<td>0.800</td>
<td>0.989</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Q235A</td>
<td>Q195</td>
<td>0.901</td>
<td>0.859</td>
<td>0.945</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Q215B</td>
<td>Q195</td>
<td>0.880</td>
<td>0.859</td>
<td>0.901</td>
<td></td>
</tr>
<tr>
<td>S45C</td>
<td>45Mn</td>
<td>45Mn</td>
<td>0.906</td>
<td>0.923</td>
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<td></td>
</tr>
<tr>
<td></td>
<td>45</td>
<td>45</td>
<td>0.904</td>
<td>0.923</td>
<td>0.885</td>
<td></td>
</tr>
<tr>
<td></td>
<td>50Mn</td>
<td>50</td>
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<td>0.919</td>
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<tr>
<td></td>
<td>50</td>
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<td>00C18Ni10</td>
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<tr>
<td>SUS631(RH950)</td>
<td>0Cr17Ni7Al</td>
<td>0Cr17Ni7Al</td>
<td>0.960</td>
<td>0.924</td>
<td>0.997</td>
<td></td>
</tr>
<tr>
<td>SUH310</td>
<td>1Cr25Ni20Si2</td>
<td>1Cr25Ni20Si2</td>
<td>0.863</td>
<td>0.790</td>
<td>0.942</td>
<td></td>
</tr>
</tbody>
</table>

4. Summary

The conception of DMS is developed to actualize data matching between two or more material correlated database system. The key frame of this technique is matching data set, similarity degree function and specialist rules. By this method, the primary information of a material such as composition, properties and other key characters are summarized as computational mathematic features. The conception of DMS is suitable not only steel grade database, but also can be applied to data matching and comparison between different standard for other material system.
A Computer Matching Technique for Steel Grades Comparison between Different Standards

Hang SU, Wei Han, Misako Uchida, Shigemitsu Kihara, Xiaoling Chen, Yongquan Zhang

2006.1 Japan

1. Introduction

- Global sourcing
  - The age of global economic integration
  - material procurement for manufactory industry
  - Requires
    - databases for various material standards
    - A comparative information system of world material standards
    - techniques to process the material comparing and matching between standard from different countries
1. Introduction

- Existing work
  - handbooks based on specialists experience
  - Web base table

- Problem
  - Not all things considered
  - Difficult to refresh and maintain

- Recently years, artificial intelligence techniques were applied in data mining and knowledge discovery
  - pattern recognition
  - artificial neural networks

- In this paper, a computer matching technique (DMS) has been put forward for steel grades auto comparison between different standards.
  - DMS (Data Matching Subsystem) is designed to actualize data matching automatically between two or more material correlated database system.
1. Introduction

- By DMS, the basic information of a steel grade was summarized as several mathematic features.
  - Compositions
  - Properties
  - Applications
  - Shapes
  - Special properties
  - Delivery states

- Key conception: *Similarity Degree*
  - *Similarity Degree* between different steels were calculate based on the above features
  - With conception of *Similarity Degree*, the auto matching and auto comparing for steel grade between different standard can be actualize.
2. Principle

- The planning application of DMS in steel grade matching between different standards.

![Diagram showing DMS connections with various steel databases including ASTM, GB/YB, DIN, JIS, ISO, and Others.]

2. Principle

- The key frame of a typical DMS
  - Matching Data Set
  - Similarity Degree Function
  - Knowledge Base.
2.1. Matching Data Set

- Matching data set defines a standardized data set that abstract the primary features of a kind material
  - main composition
  - mechanical properties
  - other features (keywords)

- For alloyed steel database, the matching data set can be summarized as a composition-property matrix and a keywords matrix as follows

\[
X_{n \times N} = \begin{bmatrix}
X_{11} & X_{12} & \ldots & X_{1N} & P_{11} & P_{12} & \ldots & P_{1M} \\
X_{21} & X_{22} & \ldots & X_{2N} & P_{21} & P_{22} & \ldots & P_{2M} \\
M & M & \ldots & M & M & M & \ldots & M \\
X_{n1} & X_{n2} & \ldots & X_{nN} & P_{n1} & P_{n2} & \ldots & P_{nM}
\end{bmatrix}
\]

- \( n \) - the total number of steels in database;
- \( N \) - the number of element
- \( M \) - the number of property indexes.
2.1. Matching Data Set

\[
K_{nx4} = \begin{bmatrix}
k_1^{\text{shape}} & k_1^{\text{app}} & k_1^{\text{sapp}} & k_1^{\text{deliv}} \\
k_2^{\text{shape}} & k_2^{\text{app}} & k_2^{\text{sapp}} & k_2^{\text{deliv}} \\
M & M & M & M \\
k_n^{\text{shape}} & k_n^{\text{app}} & k_n^{\text{sapp}} & k_n^{\text{deliv}}
\end{bmatrix}
\]

- \( n \) - the total number of steels in database;
- \( k_{\text{shape}} \) - the shape keywords
- \( k_{\text{app}} \) - the application keywords
- \( k_{\text{sapp}} \) - the specious application keywords
- \( k_{\text{deliv}} \) - the delivery state keywords

2.2. Similarity Degree Function

- Similarity degree function defines the algorithms to calculate similarity degree between two matching data set.
Example of Similarity Degree Function

- **Radar graph**
  - $S_A$ — The area of steel $A$
  - $S_i$ — The area of steel $i$
  - $S_{Ai}$ — The area of steel $A$ overlapped with steel $i$

- The composition similarity degree (DSC) between steel $A$ and $i$ defined as
  \[
  DSC_i = \frac{2S_{Ai}}{S_A + S_i}
  \]

- The similarity degree of properties (DSP) can be calculated in a similar way.

2.3. Knowledge Base

<table>
<thead>
<tr>
<th>Steel Name</th>
<th>C</th>
<th>Si</th>
<th>Mn</th>
<th>P</th>
<th>S</th>
<th>Ni</th>
<th>Cr</th>
<th>Cu</th>
</tr>
</thead>
<tbody>
<tr>
<td>SS330(SS34)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SS400(SS41)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SPHD</td>
<td>≤0.10</td>
<td>≤0.5</td>
<td>≤0.04</td>
<td>≤0.04</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SPHC</td>
<td>≤0.15</td>
<td>≤0.6</td>
<td>≤0.05</td>
<td>≤0.05</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SPHE</td>
<td>≤0.10</td>
<td>≤0.5</td>
<td>≤0.03</td>
<td>≤0.035</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>S10C</td>
<td>0.08~0.13</td>
<td>0.15~0.35</td>
<td>0.3~0.6</td>
<td>≤0.03</td>
<td>≤0.035</td>
<td>≤0.2</td>
<td>≤0.2</td>
<td>≤0.3</td>
</tr>
<tr>
<td>S15C</td>
<td>0.13~0.18</td>
<td>0.15~0.35</td>
<td>0.3~0.6</td>
<td>≤0.03</td>
<td>≤0.035</td>
<td>≤0.2</td>
<td>≤0.2</td>
<td>≤0.3</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>SteelName</th>
<th>Thickness</th>
<th>Rel</th>
<th>Rm</th>
<th>A</th>
</tr>
</thead>
<tbody>
<tr>
<td>SS330 (SS34)</td>
<td>5~16</td>
<td>≥205</td>
<td>330~430</td>
<td>≥21</td>
</tr>
<tr>
<td>SS400 (SS41)</td>
<td>&lt;5</td>
<td>≥245</td>
<td>400~510</td>
<td>≥21</td>
</tr>
<tr>
<td>SPHC</td>
<td>4~</td>
<td>≥275</td>
<td>≥31</td>
<td></td>
</tr>
<tr>
<td>SPHD</td>
<td>1.6~2</td>
<td>≥275</td>
<td>≥32</td>
<td></td>
</tr>
</tbody>
</table>
2.3. Knowledge Base

- For example
  
  **Rule1: Data Range Appointment**
  
  When the value of an element or a property (marked as X) has been given as “a ~ b”, then appointment typical value of X as follows:
  
  \[ X = \frac{a+b}{2} \]

  **Rule5: Micro-Alloyed Elements Appointment**
  
  Consider about two steels A and B, when both of them has one or more micro-alloyed elements (Nb, V, Ti, Al), and the values less than 0.05, then the typical value of these elements appointment as follows:
  
  \[ X_A = X_B \]

3. Development and application

- Original program has been developed to actualize the material matching between different steel database.

- Example application: China-Japan steel grades exchange database
  
  Co-worked by CISRI, IHI, AT&M, BM.
Program Structure

There are 6 main modules and 2 main frames in the program.

1. **ModMain**: Main module, define global variable, data structure, call for user interface.
2. **ModDatabase**: Data I/O interface, read data from JIS database and GB database.
3. **ModDSFunction**: Functions base, define all DMS functions and standardization function.
4. **ModKnowledge**: Knowledgebase, define specialist rules for composition and properties data.
5. **ModMatching**: Allotting the matching progress, such as calling for data and specialist rules, processing data standardization, calculating D\_SP and DSC.
6. **ModTable**: Create tables and report forms.
7. **frm_Main**: User interface, input steel name, set up options, output results in tables and report forms.
8. **frm_Find**: Searching from a database with inputted keywords.

Comparison of handbook result and DMS matching result between several JIS steel and GB steel.

<table>
<thead>
<tr>
<th>JIS steel</th>
<th>Handbook result</th>
<th>Matched GB steel</th>
<th>DMS result (DS(\geq)0.85)</th>
<th>DS= SQRT(DSC\times DSC)</th>
<th>DSC</th>
<th>DSP</th>
</tr>
</thead>
<tbody>
<tr>
<td>SS330(SS34)</td>
<td>Q195 Q215A Q215B</td>
<td>Q215A</td>
<td>0.92</td>
<td>0.859</td>
<td>0.989</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Q215B</td>
<td>0.89</td>
<td>0.800</td>
<td>0.989</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Q235A</td>
<td>0.90</td>
<td>0.859</td>
<td>0.945</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Q195</td>
<td>0.88</td>
<td>0.859</td>
<td>0.901</td>
<td></td>
</tr>
<tr>
<td>S45C</td>
<td>45Mn 45 50Mn</td>
<td>45Mn</td>
<td>0.91</td>
<td>0.923</td>
<td>0.890</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>45</td>
<td>0.90</td>
<td>0.923</td>
<td>0.885</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>50Mn</td>
<td>0.91</td>
<td>0.918</td>
<td>0.900</td>
<td></td>
</tr>
</tbody>
</table>

The DMS gives not only correct result, but also more detail information than handbook data.
4. Summary

- The conception of DMS is developed to actualize data matching between two or more material database system.
- The key frame of this technique is matching data set, similarity degree function and specialist rules.
- The conception of DMS is suitable not only steel grade database, but also can be applied to other material system.

Thanks!
Development of Optimum Material Selection Program for various equipments

Shigemitsu Kihara, Best Materia Co.

1. Introduction

Material data is essentially needed in every process of design, fabrication, operation and maintenance of plant, equipment and machine. Material database includes material standards, design standard (Allowable stress etc.), mechanical properties, corrosion resistance, physical properties, processing (Welding, Machining, Casting, Forging) abilities, failure mechanism, mode & cases and cost. Application programs in these processes are required for effective utilization of material database. The relation between the process and database is shown in Fig 1 (slide 2). The selection programs for optimum material in design, processing in works and maintenance method in users of equipments are discussed here.

2. Optimum Material Selection program

The optimum material is selected in the consideration of material properties, cost and availability. The desirable procedures of material selection are as follows,

Step 1: To fix design condition (applied stress, temperature and environment)
Step 2: To convert from the design condition to material requirement
Step 3: To search the material in data base fitting the requirement
Step 4: To select the optimum material in addition of information about cost and availability

The Step 2 is the key step to make good selection and should be done by corporation of designer and material engineer. The material database should be international. The information about cost and availability must be supplied by material makers as updated data. As examples material selection programs for boiler and heat exchanger tubes are mentioned below.

2.1 Boiler tube

The flow of material selection for boiler tube is shown in Fig 2 (slide 6). Usually thermal power boiler is designed by design code like ASME Boiler & Pressure Vessel code. The design code shows allowable stresses at design temperatures and temperature limit for each material. When the steam temperature is designated, usable materials are screened and the allowable stresses (Sa) at the temperature for screened materials are suggested. Wall thickness (t) is calculated by equation (1),

\[ t = \frac{P D}{2S_a} \]  

P: steam pressure, D: outer diameter of tube
When fuel (coal, oil, natural gas etc) is designated, corrosion rates are suggested for screened materials from corrosion database. The corrosion allowance is calculated by the corrosion rate data and the total thickness is fixed. The costs for tubes of screened materials are obtained by the cost information from material makers. Then the priority of material is fixed. Final selection is done by the designer under consideration of processing ability and cost negotiation with material makers.

2.2 Heat exchanger tube

The flow of material selection for boiler tube is shown in Fig 3 (slide 7). The material is selected to avoid stress corrosion cracking using critical curves for materials in the temperature – Cl⁻ content diagram.

3. Other material database and application programs

3.1 Optimum process condition selection program

The program gives optimum conditions for processes (like welding and heat treatment) from the database of process ability of materials. See slide 8.

3.2 Optimum maintenance method selection program

Maintenance should be planned by following steps; (see slide 9-12)

1) Screen failure mechanism & mode
2) Suggests inspection method and residual life evaluation

3.3 Quality evaluation

The quality is always identified in materials specified by same standard. The example is shown in slide 13 and 14. High S content is usually allowed in standards of carbon steels. But actual S content is very low in high quality steels (high impact strength). Quality information is important for reliable use of materials.

4. Summary

Followings are summarized.

1) Material database including various information (mechanical, physical and chemical properties, standard, failure, cost, quality etc) exist separately in various areas and not utilized effectively.

2) Followings are needed for effective utilization of material database;
   - to clarify where the material database is existing.
   - to develop programs (software) for applying the database to purpose properly, like programs for selection of optimum material, processing and maintenance

3) International collaboration is necessary to realize the optimum material selection system.
Development of Optimum Material Selection Program for Various Equipments

Shigemitsu Kihara
Best Materia Co., Ltd
s-kihara@b-mat.co.jp

Material Database
- Failure mechanism & case, Standard, Design standard (Allowable stress, etc.), Mechanical properties, Corrosion resistance, Physical properties, Process (Welding, Machining), Testing method, Cost

Fig 1 Material flow in the life of equipment, material database and programs
What is Material Data

- Material standard (Chemical composition, Minimum strength, Tolerance, Manufacturing process)
- Design standard (Allowable stress etc.)
- Mechanical properties (Tensile, Impact, Fatigue, Creep)
- Corrosion resistance
- Physical properties
- Processing (Weldability, Machinability, Casting, Forging)
- Failure mechanism & cases

Program for optimum material selection

Programs are prepared for parts: Parts of pressure vessels, Bolt, Gear etc.

Input

Required conditions
Shape, Design code, Applied pressure (Stress state & value), Applied temperature,
Atmosphere exposed (Corrosion atmosphere)

Output

Candidate material names, Size (Thickness), Cost and Priority

Data needed

Material standard, Design standard (Allowable stress etc.)
Mechanical properties, Corrosion resistance, Physical properties
Processing (Weldability, Machinability, Casting, Forging)
Failure mechanism & cases, Cost
**Program for optimum material selection**

**What is Optimum Material**

**Highest reliability & lowest cost**

Satisfy specification but not over

Specification (Required properties) must be suitable

<table>
<thead>
<tr>
<th>Required properties</th>
<th>Specified by</th>
</tr>
</thead>
<tbody>
<tr>
<td>Minimum tensile strength</td>
<td>Material standard</td>
</tr>
<tr>
<td>Toughness</td>
<td>Extra chemical composition and heat treatment (S content for steel)</td>
</tr>
<tr>
<td>Fatigue, Creep strength</td>
<td>Extra specification</td>
</tr>
<tr>
<td>Corrosion resistance</td>
<td>Chemical composition</td>
</tr>
<tr>
<td>Weldability</td>
<td>Chemical composition</td>
</tr>
</tbody>
</table>

**Formula**

\[ t = \frac{PD}{2Sa}, \]

- \( t \): wall thickness
- \( P \): pressure
- \( D \): tube diameter
- \( Sa \): allowable stress

**Example table of final output of the program**

<table>
<thead>
<tr>
<th>Material name</th>
<th>Wall thickness (mm)</th>
<th>Cost (¥/m)</th>
<th>Priority</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>10</td>
<td>1,000</td>
<td>1</td>
</tr>
<tr>
<td>B</td>
<td>12</td>
<td>1,200</td>
<td>2</td>
</tr>
<tr>
<td>C</td>
<td>11</td>
<td>1,400</td>
<td>3</td>
</tr>
</tbody>
</table>

**Fig 2 Flow of material selection of boiler tube**
Input
Cl- contents of water: 50 ppm
Tube skin temperature: 70 °C
Deposit: No

Output
Material recommended: Dual Phase Stainless Steel
Cost: ¥ X /m
Makers: A, B, C

Database

![Graph showing critical curves of Cl- SCC for various steels.](image)

Fig 3 Flow of optimum material selection for heat exchanger tube

**Program** for selection of optimum process condition

The program suggests suitable items for each process on specified material.

<table>
<thead>
<tr>
<th>Process</th>
<th>Items suggested</th>
</tr>
</thead>
<tbody>
<tr>
<td>Welding</td>
<td>Method, Rod, Current range, Interlayer temperature range</td>
</tr>
<tr>
<td>Heat treatment</td>
<td>Temperature range, Keep time, Heating/cooling rates</td>
</tr>
</tbody>
</table>
Program for selection of optimum maintenance condition

### Input
- Material used
- Service conditions (Temperature, Stress state & value, Atmosphere service time)

### Output
- Failure mechanism & mode anticipated
- Inspection method
- Life evaluation method
- Database & Program
- Failure mechanism & mode database
- Maintenance planning

### Failure mode & mechanism database

<table>
<thead>
<tr>
<th>Failure mode</th>
<th>Failure mechanism (number)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thinning</td>
<td>Wear (6)</td>
</tr>
<tr>
<td></td>
<td>Erosion (7)</td>
</tr>
<tr>
<td></td>
<td>General corrosion (39)</td>
</tr>
<tr>
<td>Local</td>
<td>Pitting (10)</td>
</tr>
<tr>
<td></td>
<td>Galvanic corrosion (3)</td>
</tr>
<tr>
<td></td>
<td>Crevice corrosion (3)</td>
</tr>
<tr>
<td>Cracking</td>
<td>Fatigue (7)</td>
</tr>
<tr>
<td></td>
<td>Creep (3)</td>
</tr>
<tr>
<td></td>
<td>Stress corrosion cracking (18)</td>
</tr>
<tr>
<td>Deformation</td>
<td>Creep</td>
</tr>
<tr>
<td>Degradation</td>
<td>Embrittlement (17)</td>
</tr>
<tr>
<td></td>
<td>Degradation of corrosion resistance</td>
</tr>
<tr>
<td></td>
<td>Degradation of strength (2)</td>
</tr>
</tbody>
</table>

More than 100 mechanisms are included.
**Program** for selection of optimum maintenance condition

**Example 1 (Heater)**

**Input**
- Material used: Carbon steel
- Operating temperature: 450 °C
- Operation time: 20 years

**Database/Program**
- Failure mechanism & mode screening program
  - Graphitization
  - Rapture

**Database**
- Inspection methods for failure mechanism & mode

**Conclusion**
- Inspection method recommended: Microstructural observation
- Countermeasure recommended, if detected: Change material to Cr-Mo steel

**Program** for selection of optimum maintenance condition

**Example 2 (Boiler tube)**

**Input**
- Material used: 2.25Cr-1Mo steel
- Operating temperature: 550 °C
- Operation time: 20 years

**Failure mechanism & mode anticipated**
- Creep rapture

**Database**
- NIMS Creep data sheets
- NIMS standard microstructure after high temperature service

**Residual life evaluation**
- Creep test on sampled test pieces
- Microstructure and void observation

**Conclusion**: Continuous use or Replace
Relation between S content and Sharpy absorbed energy, with upper limit of standard and actual content of high quality one for carbon steels

Lamella structure of low quality carbon steel
(Thickness: 16mm)

S content: 0.031mass% (Upper limit of JIS SM490A: 0.035mass%)
S<0.008mass% in high quality steel (Upper limit: 0.035mass%)
Summary

• Material database including various information (mechanical, physical and chemical properties, standard, failure, cost, quality etc) exist separately in various areas and not utilized effectively.
• Followings are needed for effective utilization of material database ;
  • to clarify where the material database is existing.
  • to develop programs (software) for applying the database to purpose properly, like programs for selection of optimum material, processing and maintenance
• International collaboration is necessary to realize the optimum material selection system.
Material Selection Using Internet-Based Tools

Dr. Dale O. Kipp,
MatWeb Division, Automation Creations, Inc.
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Abstract:

In the past generation, computer-driven material selection has accelerated the material selection process. The dramatic increase in the speed and capacity of computers and networks, coupled with increased ease of data collection and updates, has supplanted decades of handbook-driven and experience-driven material selection. Internet databases using various business models have successfully filled roles in the material selection process. Subscription-based, government supported, and free Internet databases have all found roles with today’s tech-savvy engineers. MatWeb’s business model (broad array of materials, advertising supported, moderately high level of search tools) has made it the busiest web site for materials data, serving over 22,000 users each weekday. This talk will examine the roles and capabilities of MatWeb and other Internet materials databases in the material selection process.
Material Selection Using Internet-Based Tools

Dr. Dale O. Kipp,
MatWeb Division, Automation Creations, Inc.

MITS Meeting 2006
Tokyo Japan
January 20, 2006

Introduction

• In the past generation, computer-driven material selection has accelerated the material selection process. The dramatic increase in the speed and capacity of computers and networks have made reversed decades of handbook-driven and experience-driven material selection.

Processor speed + storage capacity + network access = Internet-driven material selection
Data Collection

- Aside from technology, funding mechanisms were also needed to bring about new routes to materials selection:
  - Subscriptions/payments from users
  - Government funding
  - Free to users
    - Advertising pays for content
    - Seller/producer uses as promotional vehicle

Different databases for different purposes

- Breadth – The number of unique materials available within the material selection tools. A broad database will cover all materials within metals, polymers, and ceramics. Most necessary in the early stages of material selection.

- Depth – The level of detail available for a given material. A deep database will include a wealth of graphical information, variable temperature data, cross references.
Function follows funding

- Diversity of material selection options is driven in part by diversity of business models.
  
  - A free database designed to promote copper will be narrow and not assist in the selection of nickel alloys
  - A free database is not expected to have as much depth of information as one that relies on payments from users

Property-Based Searches

- This talk will focus on quantitative material selection criteria.

- Google or other text-based searches can be important early in the selection process of materials when a specific application or qualitative attribute can be described in succinct, specific text.
<table>
<thead>
<tr>
<th></th>
<th>Free</th>
<th>Subscription</th>
</tr>
</thead>
<tbody>
<tr>
<td>Comprehensive</td>
<td>MatWeb AZOM</td>
<td>Granta Design/ASM International</td>
</tr>
<tr>
<td>Focused</td>
<td>P/M Database Fotofab GE Plastics NIMS</td>
<td>IDES Key to Steel</td>
</tr>
</tbody>
</table>
Powder Metallurgy Property Database

- Typical Results Set:

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe-0893</td>
<td>Ferrous</td>
<td>91 of 93</td>
<td>569</td>
<td>520</td>
<td>680</td>
<td>140000</td>
<td>167000</td>
<td>217</td>
</tr>
<tr>
<td>Fe-0589C2D-0625</td>
<td>Ferrous</td>
<td>35 of 217</td>
<td>450</td>
<td>410</td>
<td>500</td>
<td>140000</td>
<td>170000</td>
<td>150</td>
</tr>
<tr>
<td>Fe-0589C2D-0625</td>
<td>Ferrous</td>
<td>33 of 217</td>
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<td>410</td>
<td>500</td>
<td>140000</td>
<td>170000</td>
<td>150</td>
</tr>
<tr>
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<td>23 of 100</td>
<td>430</td>
<td>390</td>
<td>500</td>
<td>140000</td>
<td>190000</td>
<td>160</td>
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<tr>
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<td>Ferrous</td>
<td>17 of 99</td>
<td>380</td>
<td>340</td>
<td>500</td>
<td>140000</td>
<td>190000</td>
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<tr>
<td>Fe-0589C2D-0625</td>
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<td>15 of 74</td>
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<td>160000</td>
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<tr>
<td>Fe-0589C2D-0625</td>
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<td>14 of 61</td>
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<td>240</td>
<td>420</td>
<td>140000</td>
<td>160000</td>
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<td>12 of 59</td>
<td>230</td>
<td>190</td>
<td>380</td>
<td>140000</td>
<td>160000</td>
<td>88</td>
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<tr>
<td>Fe-0589C2D-0625</td>
<td>Ferrous</td>
<td>12 of 59</td>
<td>230</td>
<td>190</td>
<td>380</td>
<td>140000</td>
<td>160000</td>
<td>88</td>
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<td>140</td>
<td>340</td>
<td>140000</td>
<td>160000</td>
<td>50</td>
</tr>
</tbody>
</table>

- X-Y Comparison plots also available.

NIMS Databases

- Much of the data is measured at NIMS
- Several databases available:
  - PoLyInfo
  - Metals and Alloy Database
    - Structural Materials Database
    - Nuclear Materials Database
    - Welding Database
    - Pressure Vessel Materials
  - Superconductivity Database
    - Superconducting Materials
    - High Magnetic Field Engineering
  - Basic Properties Database
NIMS Databases

- Sample of Creep data sheets available within Structural Materials Database

<table>
<thead>
<tr>
<th>No.</th>
<th>Data Sheet Description</th>
<th>Year</th>
</tr>
</thead>
<tbody>
<tr>
<td>1B</td>
<td>DATA SHEETS ON THE ELEVATED-TEMPERATURE PROPERTIES OF 1Cr-0.5Mo STEEL TUBES FOR BOILERS AND HEAT EXCHANGERS (STBA 22)</td>
<td>1996</td>
</tr>
<tr>
<td>2B</td>
<td>DATA SHEETS ON THE ELEVATED-TEMPERATURE PROPERTIES OF 1.25Cr-0.5Mo-Si STEEL FOR BOILER AND HEAT EXCHANGER SEAMLESS TUBES (STBA 23)</td>
<td>2001</td>
</tr>
<tr>
<td>3B</td>
<td>DATA SHEETS ON THE ELEVATED-TEMPERATURE PROPERTIES OF 2.25Cr-1Mo STEEL FOR BOILER AND HEAT EXCHANGER SEAMLESS TUBES (STBA 24)</td>
<td>1996</td>
</tr>
<tr>
<td>4B</td>
<td>DATA SHEETS ON THE ELEVATED-TEMPERATURE PROPERTIES OF 18Cr-9Ni STAINLESS STEEL FOR BOILER AND HEAT EXCHANGER SEAMLESS TUBES (SUS 304H TB)</td>
<td>1996</td>
</tr>
<tr>
<td>5B</td>
<td>DATA SHEETS ON THE ELEVATED-TEMPERATURE PROPERTIES OF 18Cr-10Ni-Ti STAINLESS STEEL FOR BOILER AND HEAT EXCHANGER SEAMLESS TUBES (SUS 321H TB)</td>
<td>1997</td>
</tr>
</tbody>
</table>

- Each datasheet is extremely detailed with creep data and supporting information – dozens of pages VERY DEEP

MatWeb

- Database Business Case – Attract potential customers for photolithography processing of certain metal strip products
- Product Selection Case – 2000 Metal data sheets plus search & compare tools
  - Web site’s data and tools licensed from MatWeb, including some capabilities that are subscription-only on MatWeb
GE Plastics

- Database Business Case – Attract potential customers for premium thermoplastics
- Product Selection Case – 2300 Thermoplastic data sheets plus search & compare tools
  - Web site’s data and tools licensed from IDES, including some capabilities that are subscription-only on IDES

IDES

- Most comprehensive plastics database – 60,000 data sheets reported
- Property-based search and compare capabilities
- Alternative resin finder
- Multi Point Search
  - Property-based search starts at US$499/yr
  - Free access to data sheets only (without search tools)
Key to Steel

- Steel only
- 44,000 cross references, 20,000 include data sheet
  - US$295/year

AZOM
(A to Z of Materials)

- Database Business Case: Advertising supported, currently over 20,000 users per day
- Product Selection Case: Free. AZOM’s strength lies in articles, news, and journals.
- Property-based search allows choice of two properties from list of 40, in combination with keywords. Broad selection of data sheets, including metals, polymers, and ceramics. Total data sheet count (?Many hundreds?)
- Data from manufacturer or handbook/literature/professional society; source listed
• Database Business Case: Advertising supported, currently over 20,000 users per day
• Product Selection Case: Free (additional selection and tools for US$75/year). Focus of the web site is materials selection. Very broad database with advanced search tools.

• Property-based search allows choice of three physical properties from lists of 90, in combination with categories or alloy compositions. Broad selection of data sheets, including metals, polymers, and ceramics. Total data sheet count > 54,000. Average data sheet has 18 physical property data points.
• Data from manufacturer (>80%) or handbook/literature/professional society; source listed
• Affiliated with ASM International
• CES Selector – features systematically complete data sheets (no holes)
• Additional databases available to add breadth (Polymers from CAMPUS and IDES; EcoSelector)
• Cost not quoted on Web site

CES Selector from Granta Design
• Two-Dimensional Graphical Selection Tools
ASM International

- Alloy Finder
- 105,000 alloy designations; 15,000 data sheets
- Graphical information adds to depth
- US$1500/year

Summary

- Today’s engineers enjoy a large variety of material selection tools available from their desktop.
- Different business goals and different material selection goals create an environment in which many different databases can thrive.
Thanks

- Thanks to Dr. Koichi Yagi and NIMS for the invitation to speak here.

- Questions?

Dale Kipp
E-mail dale.kipp@matweb.com
Landolt-Börnstein in the electronic age: a collection of “Numerical Data and Functional Relationships in Science and Technology” going online

Rainer Poerschke and Werner Martienssen
Landolt-Börnstein at Springer-Verlag, Berlin (RP) and
Physikalisches Institut der Johann Wolfgang Goethe Universität, Frankfurt am Main (WM)
Rainer.poerschke@springer.com, martienssen@physik.uni-frankfurt.de

1. Introduction

Landolt Börnstein was founded by the scientists Hans Landolt and Richard Börnstein with Julius Springer in Berlin 1883, i.e. more than 120 years ago with a single handbook on physical data. Six editions of the handbook followed until an open “New Series” was started in the sixties to collect data in a more continuous way and to change to fields of new activities faster than it was possible in the past.

The Landolt-Börnstein collection is structured into eight groups:

- Group I: Elementary particles and nuclei,
- Group II: Molecules and radicals,
- Group III: Condensed matter,
- Group IV: Physical chemistry,
- Group V: Geophysics,
- Group VI: Astrophysics,
- Group VII: Biophysics,
- Group VIII: Advanced technology and materials.

The larger Groups I, II, III and IV are further divided into a number of “Sections”

Since 1996 CD-ROMs were produced aside to the printed handbooks allowing for fulltext search and easy navigation due to hyperlinks. Today the “New Series” spans more than 300 printed (sub)volumes and 140 CD-ROMs.

In the year 2000 a first internet-version of Landolt-Börnstein was opened up giving free entrance to all content published until 1990. 10,000 users registered immediately and more than 2 million downloaded documents were counted in this special year of free access.

Though a survey showed the users to like the electronic presentation of the LB-content and the new fulltext functionalities Springer and the Landolt-Börnstein group was ambitious to develop even better electronic versions. The next version went online in 2002 and in 2003 Springer completely changed it’s server from a file system to a database system, which allows better administration functionalities for an increasing content and increasing number of users.

Meanwhile Springer offers more than 1400 journals and a large number of book series including the Landolt-Börnstein Collection, online. The total number of real document downloads was about 25 million in the year 2005 and is moving upwards steadily.

2. State of the Landolt-Börnstein online collection

landolt-boernstein.com, the homepage on springeronline.com is the starting point for users, whereas the content (pdf-files) are on springerlink.com. From the homepage one can navigate to the groups and find the sections and titles of interest easily. One click further leads to short descriptions of volumes and subvolumes and to the tables of contents. Up to this point open access is provided. To download a document on Springerlink as a next step is for licensed users only (IP-address-control or password), single documents can also be bought like journal articles using a credit card.

From the homepages landolt-boernstein.com indexes help to navigate fast to chemical substances (organic and inorganic) and their properties. The organic Scidex-database-index allows graphical structure search. In html-format organic and inorganic index give an easy access directly to the
LB-documents. Substance indexes are also provided as pdf-indexes, which can be downloaded on the PCs of the users and stay there for permanent help. A Comprehensive Index (Keyword Index) is available the same way. This index in the moment runs only until the year 1997, an updated version is in preparation.

3. Future Prospects
Redetermining the fields of our Science Data Collection according to the users needs is done continuously is done by surveys and discussions with our editors, authors and of course users. Quality maintenance in the electronic world of data and metadata is an important task. For this we have an editorial office with five scientists and five assistants, who work with the authors and editors to reach perfection of the manuscripts before publication and produce the necessary metadata in xml (A++)). Indexes for each volume are also produced there in cooperation with chemists and database developers (LCI-publisher, Hamburg).

A complete relaunch of Landolt-Börnstein on the so-called Springer Major Reference Platform as a “Knowledge System” is scheduled to be opened in May of 2006.

4. Summary
The Landolt-Börnstein principle “Extracting critically selected scientific data from the literature and embedding these data into the scientific context by experts in the respective field” has not changed over a long period of more than 120 years.
New electronic publication modes facilitate usage of the giant data collection (38,000 documents) at the working computer. Navigation and search is much easier compared to the printed version due to Links, Indexes and an up to date search engine. The targets of the data collection are adjusted according to the feedback of our users more frequently than it was possible in the past.
Landolt-Börnstein in the electronic age:
the collection of „Numerical Data and Functional Relationships in Science and Technology“ going online

Rainer Poerschke¹) and Werner Martienssen²)

¹) Executive Manager of LB, Springer, Berlin/Darmstadt
²) Editor-in-chief of LB, Physics Dept. of the Johann Wolfgang Goethe Univ., Frankfurt a.M.

Landolt Börnstein (LB)

- Founded in 1883 by Julius Springer and Landolt and Börnstein, both Profs. of Physical Chemistry in Berlin
- A systematic & comprehensive collection of selected and critically assessed data from original full text research journals in physical sciences & engineering, presented by more than 1,000 well-known editors & authors
- Target audience is researchers, academicians & engineers in Astrophysics, Biophysics, Physical Chemistry, Geophysics, Materials Technology and Materials Engineering
Landolt Börnstein (LB)

• Offering original research results & searchable full text contents in Materials Knowledge since the 1960’s (New Series after 6th edition)
• Equivalent to over 160.000 printed pages of valuable data in more than 30.000 document files
• Over 300.000 article downloads in 2005
• >300 volumes published up till end of 2005
  20 new volumes published 2005 (print, CD-ROM and online)
• 20 new volumes to be published in 2006,
  (4 volumes, 1 in February)

Let’s go to the LB-homepage
www.landolt-boernstein.com

www.landolt-boernstein.com, the LB-homepage

• Of general interest: Links to all LB Indexes and the volumes on “Units and Fundamental Constants”
  In addition Links to all LB-groups bundled into three “packages” do exist:
• I. Physics-package containing the LB-groups VI, VII, I and V, i.e.:
  - Astrophysics
  - Biophysics
  - Elementary Particles, Atoms and Plasmas
  - Geophysics
• II. Chemistry-package containing the LB-group II, i.e.:
  - Molecules and Radicals
• III. Materials-package containing the LB-groups VIII, III, IV, i.e.:
  - Advanced Materials and Technology
  - Condensed Matter
  - Physical Chemistry
Navigation to the content

• Start from the LB-homepage on Springeronline:
  www.landolt-boernstein.com

• Electronic catalog instead of printed one, advantage of being up to date

• Groups
  Sections
  Volumes
  Subvolumes
  Tables of contents
  pdf-documents

LB navigation in the online catalog
Group VIII Landolt-Börnstein

Energy Technologies
Laser Physics and Application
Materials
Physical Properties of Liquid Crystals
Radiological Protection

Materials

VIII/2
Powder Metallurgy Data
Subvolume A

For many applications powder metallurgy (PM) is the only way to produce economically so-called impossible materials, e.g., homogenous fine-grained immiscible materials, nanomaterials, highly alloyed segregation-free tool steels, or nickel base alloys, functionally graded materials, bonded hard materials, or rare earth hard magnets, to just name a few.

The scope of this data collection is the authoritative coverage of critically evaluated and reviewed data on physical, chemical, and mechanical properties, including information available from conference proceedings, company literature, and the internationally very different standards on PM materials, industry catalogues and brochures, research reports and scientific journals. The data collected was so extensive that the editors decided to divide the volume in two parts.

Editors: P. Beiss, R. Rothhardt, H. Warlimont

Metals and Magnets
Part 1
2003, XIV. 551 pages. ISBN: 3-540-42942-6
Table of Contents

Refractory, Hard and Intermetallic Materials
Part 2
This part provides data on refractory, hard and intermetallic materials. Physical, chemical, and mechanical properties of the materials are provided, and production, compaction, and preparation methods, as well as the various applications are thoroughly described.

Authors: G. Leichtfried, G. Sauthoff, G.E. Spriggs
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Creep Properties of Heat Resistant Steels and Superalloys
Subvolume B
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Materials

VIII/2

Powder Metallurgy Data

Subvolume A

For many applications powder metallurgy (PM) is the only way to produce economically so-called impossible materials, e.g., homogeneously fine-grained immiscible materials, nanomaterials, highly alloyed segregation-free tool steels, or nickel base alloys, functionally graded materials, bonded hard materials, or rare earth hard magnets, to just name a few.

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Editors: P. Beiss, R. Ruthardt, H. Wartime

Metals and Magnets

Part 1


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Creep Properties of Heat Resistant Steels and Superalloys

Subvolume B


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Landolt-Börnstein

GROUP VIII: Advanced Materials and Technologies

VOLUME 2

Materials

SUBVOLUME B

Creep Properties of Heat Resistant Steels and Superalloys

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Title Page

Preface

Authors

Symbols

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1.2.2 The JSME high-temperature strength data series 2

1.2.3 The long-term data series by the Iron and Steel Institute of Japan 2

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1.2.5 Report on the mechanical properties of metals at elevated temperatures by the Iron and Steel Institute of Japan 3

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1.2.7 Others 3

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2 Creep and rupture data of heat resistant steels

2.1 Carbon steels

2.1.1 0.1C steel

2.1.1.1 Introduction

This carbon steel for boiler and heat exchanger tubes is used as water tube, smoke tube, super-heater tube, air-preheater tube, etc. in boiler and as heat exchanger tube, condenser tube, catalyst tube, etc. in chemical and petrochemical industries. The carbon steels are used only at temperatures lower than 400 °C, because they have not enough creep strength for higher temperatures.

2.1.1.2 Material standards, chemical and tensile requirements

Table 1. Chemical requirements of 0.1C steel tubes, JIS STB340, ASTM A, BS3309 and DIN 2528

<table>
<thead>
<tr>
<th>Standards</th>
<th>Designation</th>
<th>Chemical composition (wt%*)</th>
<th>Std. No.</th>
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<tbody>
<tr>
<td>JIS</td>
<td>STB340</td>
<td>C: 0.18 Si: 0.35</td>
<td>G1491</td>
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<td>360</td>
<td>C: 0.17 Si: 0.30</td>
<td>A178</td>
</tr>
<tr>
<td>BS</td>
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<td>C: 0.17 Si: 0.30</td>
<td>359-2</td>
</tr>
<tr>
<td>DIN</td>
<td>St35.8</td>
<td>C: 0.17 Si: 0.30</td>
<td>17175</td>
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</tbody>
</table>

Table 2. Tensile properties of 0.1C steel tubes at room temperature, JIS STB340

<table>
<thead>
<tr>
<th>Tensile strength [N/mm²]</th>
<th>Yield strength [N/mm²]</th>
<th>Elongation [%]</th>
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<tbody>
<tr>
<td>≥340</td>
<td>≥175</td>
<td>≥20% 20 mm</td>
</tr>
<tr>
<td></td>
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<td>≥20% 20 mm</td>
</tr>
<tr>
<td></td>
<td></td>
<td>≥5% 10 mm</td>
</tr>
<tr>
<td></td>
<td></td>
<td>≥25% 10 mm</td>
</tr>
<tr>
<td></td>
<td></td>
<td>≥230</td>
</tr>
<tr>
<td></td>
<td></td>
<td>≥27%</td>
</tr>
</tbody>
</table>

erschke, W. Martienssen, 2006
Phase Equilibria, Crystallographic and Thermodynamic Data of Binary Alloys

**IV/5**

For everyone concerned with the technology and application of metals and alloys and with the development of new metallic materials, a detailed knowledge of phase equilibria is indispensable. Also, information on the thermodynamical and crystallographical data of the systems under investigation is essential, and often metastable crystalline phases as well as quasicrystalline or amorphous alloys are of interest. Volume IV/5 presents such data.

**Editor:** O. Madelung

**Author:** B. Predel

**Ac-Au ... Au-Zr**
Subvolume A


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**B-Ba ... C-Zr**
Subvolume B


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**Ca-Cd ... Co-Zr**
Subvolume C

1993. 513 figs., XXVII, 466 pages. ISBN 3-540-56072-6

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**Cr-Cs ... Cu-Zr**
Subvolume D


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---

Phase Equilibria, Crystallographic and Thermodynamic Data of Binary Alloys

**List of Alloys (ordered alphabetically)**

<table>
<thead>
<tr>
<th>Ac</th>
<th>Ag-Cr</th>
<th>Ag-Mo</th>
<th>Ag-Se</th>
<th>Al-Au</th>
<th>Al-Ho</th>
<th>Al-Pu</th>
<th>Al-Y</th>
<th>Am-Rh</th>
<th>As-Cu</th>
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<td>Ag-Si</td>
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<td>Al-In</td>
<td>Al-Re</td>
<td>Al-Yb</td>
<td>Am-Ru</td>
<td>As-Dy</td>
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<td>Ac-B</td>
<td>Ag-Cu</td>
<td>Ag-Na</td>
<td>Ag-Sm</td>
<td>Al-Ba</td>
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<td>Al-Rh</td>
<td>Al-Zn</td>
<td>Am-Sb</td>
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<td>Ag-Dy</td>
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<td>Ag-Sn</td>
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<td>Al-Rh</td>
<td>Al-Zr</td>
<td>Am-Sb</td>
<td>As-Eu</td>
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<td>Ag-Nd</td>
<td>Ag-Sr</td>
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<td>Al-La</td>
<td>Al-Ru</td>
<td>Am-M</td>
<td>As-Se</td>
<td>As-Eu</td>
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<td>Al-Sb</td>
<td>Am-Be</td>
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<td>Ag-O</td>
<td>Ag-Tb</td>
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<td>As-Si</td>
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<td>Ar</td>
<td>As-Si</td>
<td>As-Gd</td>
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<td>Ag-Gd</td>
<td>Ag-P</td>
<td>Ag-Th</td>
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<td>Al-Si</td>
<td>Ar</td>
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<td>Al-Sm</td>
<td>Am</td>
<td>Ar-Mo</td>
<td>As-Hf</td>
</tr>
<tr>
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<td>Ag-Hf</td>
<td>Ag-Tm</td>
<td>Ag-Cl</td>
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<td>Am</td>
<td>Ar-Mo</td>
<td>As-Hg</td>
</tr>
<tr>
<td>Ag-Au</td>
<td>Ag-Hg</td>
<td>Ag-Po</td>
<td>Ag-U</td>
<td>Al-Cu</td>
<td>Al-Nb</td>
<td>Al-Ta</td>
<td>As</td>
<td>As-Au</td>
<td>As-Hg</td>
</tr>
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<td>Ag-Srb</td>
<td>Ag-V</td>
<td>Al-Dy</td>
<td>Al-Nd</td>
<td>Al-Tb</td>
<td>As</td>
<td>As-B</td>
<td>As-Hg</td>
</tr>
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<td>Ag-B</td>
<td>Ag-In</td>
<td>Ag-Pr</td>
<td>Ag-W</td>
<td>Al-Er</td>
<td>Al-Ni</td>
<td>Al-Tc</td>
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<td>As-Be</td>
<td>As-Hg</td>
</tr>
<tr>
<td>Ag-Ba</td>
<td>Ag-Ir</td>
<td>Ag-Pu</td>
<td>Ag-Y</td>
<td>Al-Eu</td>
<td>Al-No</td>
<td>Al-Te</td>
<td>As</td>
<td>As-Be</td>
<td>As-Hg</td>
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Chapter

Ag-Au (Silver-Gold)
B. Predel

This chapter does not have an abstract.

Keywords:
Ag-Au (Silver-Gold)

Phase diagram

Extensive compilations concerning the phase equilibria results have been given by Hennig, Elliott and Ganszer et al. (Ref. 1) [Hennig, Elliott, Ganszer]. The solid-liquid range between the liquidus and the solidus in various Ag-Au alloys amounts to ∼2 K.

Fig. 1. Ag-Au Phase diagram.

Crystal structure

Lattice parameters of the five solid solutions are presented in Fig. 2 as a function of Au concentration [Ref. 3]. Fig. 3 gives the temperature dependence of the lattice parameter of an Ag-Au alloy with 30 at% Au [Ref. 4]. Gianone has found a short-range order in the solid solutions [Ref. 5]. Controversial results exist in this field, two studies at al. [Ref. 6] and Zemann et al. [Ref. 7]. Long-range order could not be detected [Ref. 8].
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