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New stage of MatNavi, materials database at NIMS

Toshio Ogata
National Institute for Materials Science

Masayoshi Yamazaki
National Institute for Materials Science

New stage of MatNavi, materials database at NIMS

Toshio Ogata and Masayoshi Yamazaki

Materials Information Station (MIS)
National Institute for Materials Science (NIMS)

Tsukuba, Japan

Contents

- **New MatNavi**

- **Inorganic Database (AtomWork)**
- **Interfacial Thermal Conductance Database (ITC)**
- **Computational Electronic Structure Database (CompES)**

- **Composite Design & Property Prediction System (CompoTherm)**
- **Metal Segregation Prediction System (SurfSeg)**

- **Summary**

MatNavi

NIMS

New MatNavi

MatNavi

- ✓The database server and the office was moved to Tsukuba site from Tokyo Meguro site of NIMS , on March 2010.
- ✓Updating the system and crystal structure data
  Renamed: Pauling File ⇨ Inorganic DB (AtomWork)
- ✓We've added two new databases
  Interfacial Thermal Conductance Database (ITC)
  Metallic Materials Database (Kinzoku)

Databases and application

Materials information from NIMS

Registration

Search engine

Information

Links with external organizations

Free of Charge

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

MatNavi

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No.	Database System	Data Source	
		Experimental or Calculation	Literature
1	Polymer Database (PoLyInfo)		○
2	Inorganic Database (AtomWork)		○
3	Computational Electronic Structure Database (CompES)	○	
4	Database of Promising Adsorbents for Decontamination of Radioactive Substance (READS)	○	
5	Neutron Transmutation Database (NeuTran)		○
6	Interfacial Thermal Conductance Database (ITC)	○	
7	Diffusion Database (Kakusan)		○
8	Superconducting Materials Database (SuperCon)	○	○
9	Metallic Materials Database (Kinzoku)	○	
10	CCT Diagram Database (CCTD)	○	
11	NIMS Structural Materials Data Sheet Online	○	

Database of MatNavi

MatNavi

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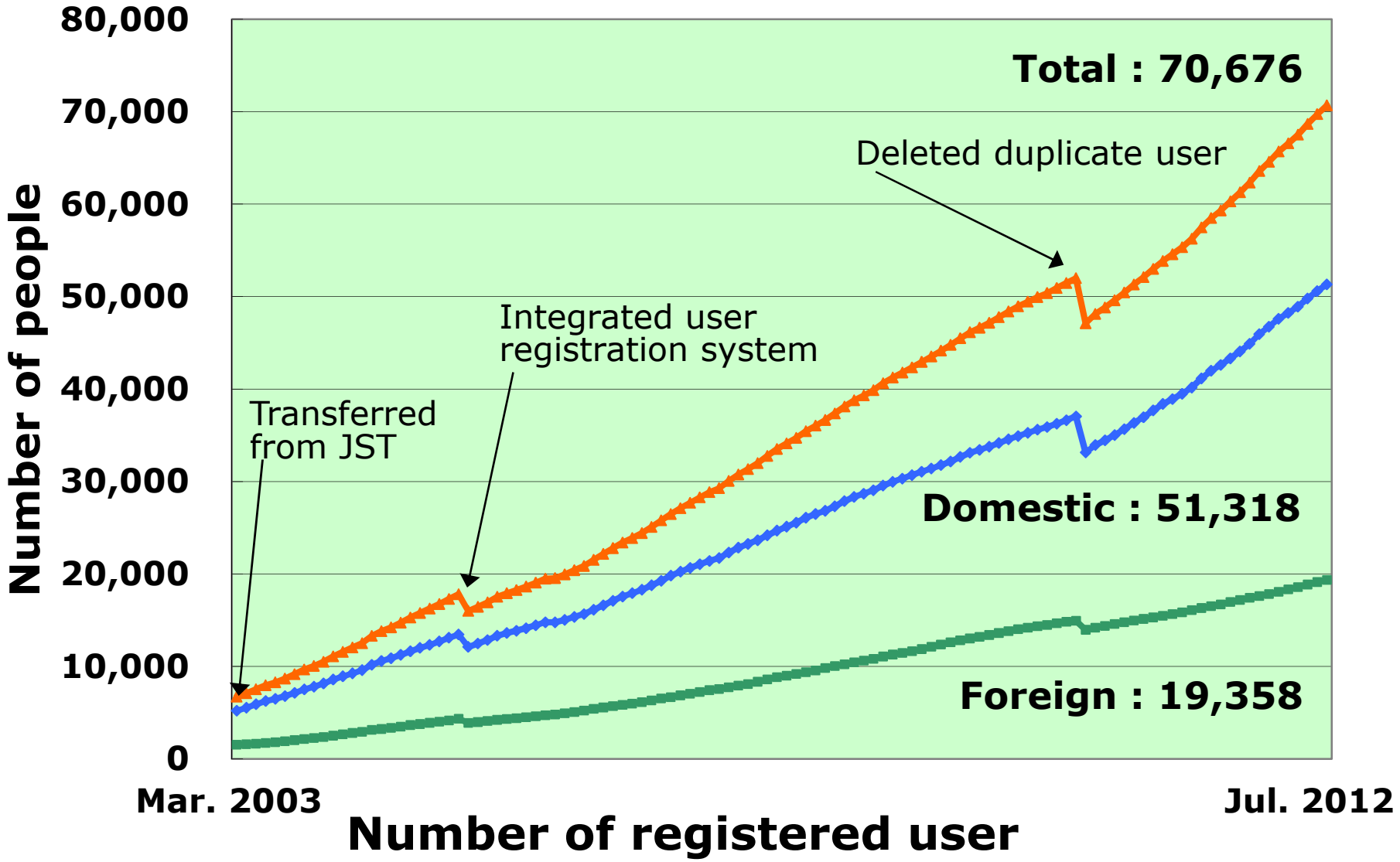

Registered users: 70,676 (Domestic: **51,318**, Foreign: **19,358**)
Locations: 141, **Organizations: 18,121** **(at Jul. 31, 2012)**

MatNavi

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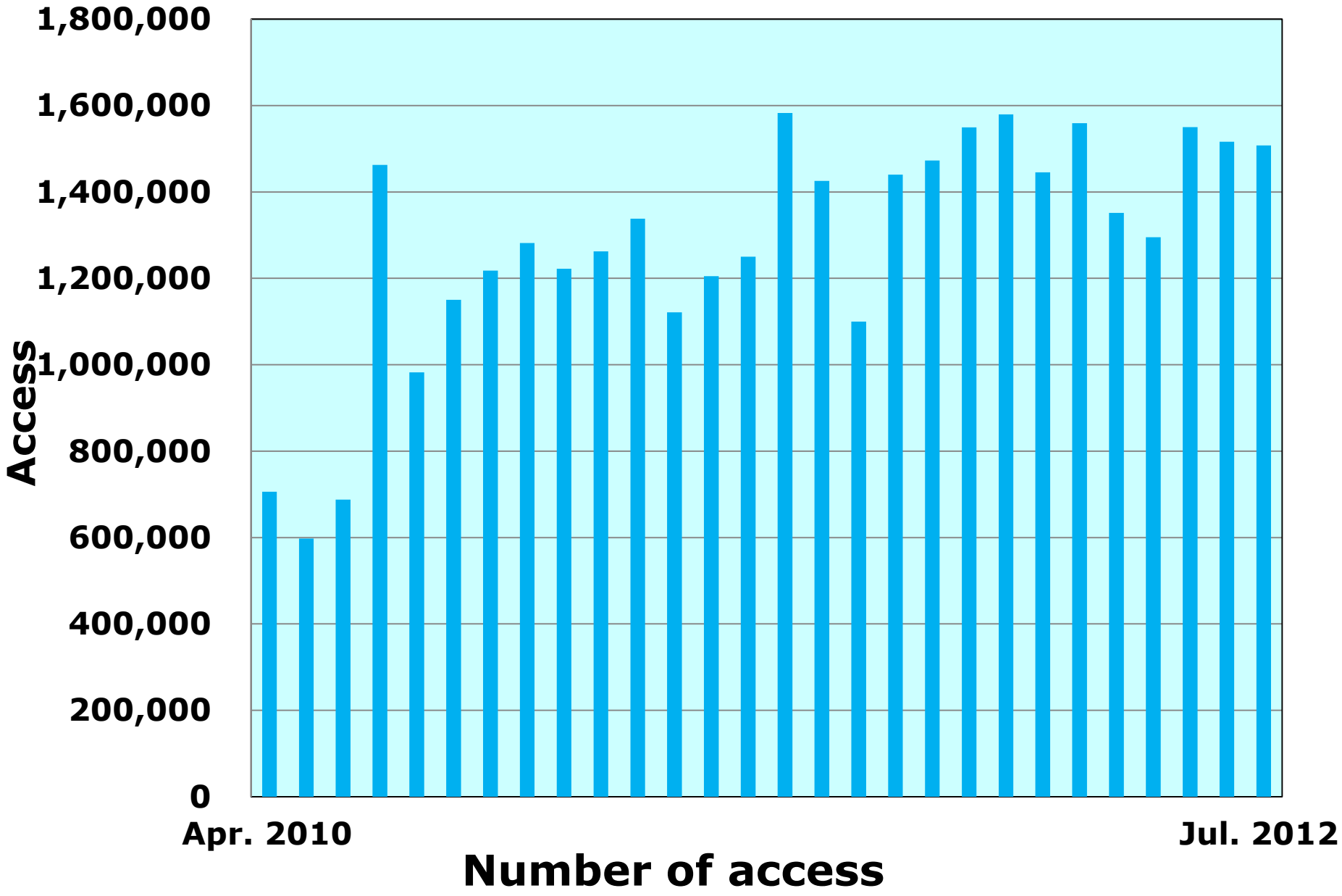

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Inorganic Database (AtomWork)

AtomWork

The Inorganic Material Database aims to cover
all basic crystal structure, x-ray diffraction, property and phase diagram data of inorganic and metallic materials from main literature sources.
You have three choices to search data:
1. "Search material" - Search materials by specifying chemical system, chemical formula, substance name, structure type (prototype), Pearson symbol or space group number.
2. "Search Materials having specified property" - Search materials by specifying property.
3. "Search phase diagrams" - Search phase diagrams by specifying chemical system.

As of July 1, 2010, the list of registered data had reached 82,000 crystal structures, 55,000 material properties and 15,000 phase diagrams.

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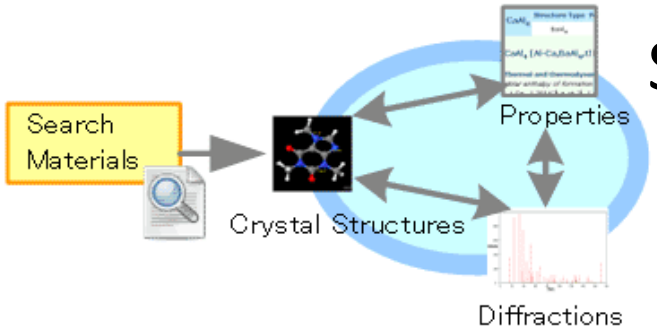
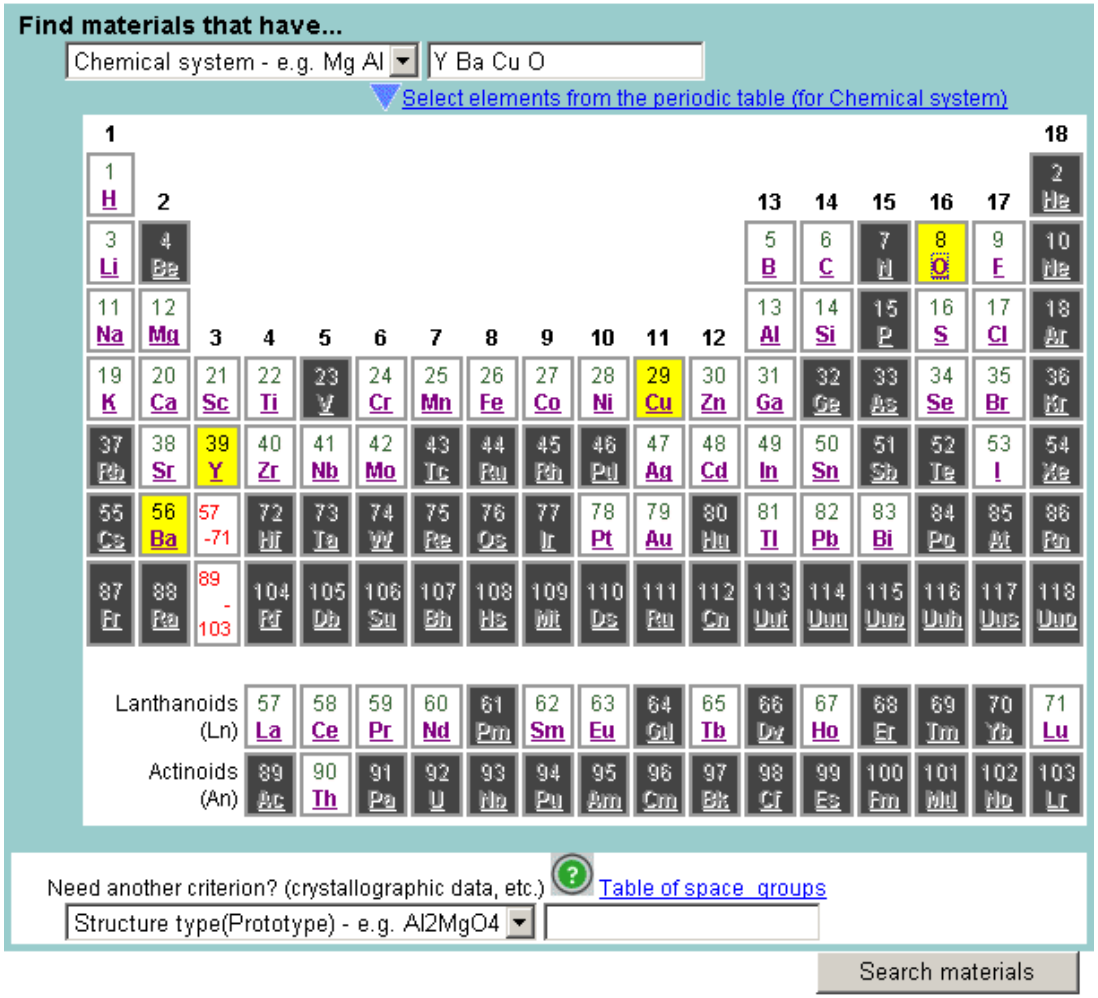
Search materials - Setting for search conditions



Selection Search sysytem



Material Search

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Details of selected material

$Ba_2Cu_3YO_6$	Structure type	Pearson symbol	Space group	No.
	$Ba_2Cu_3YO_6$	tP12	P4/mmm	123

*Standardized

J. Am. Ceram. Soc.,1995,78,,1781-1786,Mizusaki J., Tagawa H., Hayakawa K., Hirano K.

Preparation

Synthesis No data.

Starting materials No data.

Crystal Structure | X-ray Diffraction | Properties

Crystal Structure (Published)

Niggli-reduced cell

Crystallographic data

Cell parameters a = 0.386 nm, b = 0.386 nm, c = 1.184 nm, α = 90 ° , ß = 90 ° , γ = 90 °

Cell volume 0.17641 nm^3

Crystal Structure (Standardized)

Crystallographic data

Cell parameters a = 0.386 nm, b = 0.386 nm, c = 1.184 nm, α = 90 ° , ß = 90 ° , γ = 90 °

Cell volume 0.1764 nm^3

Cell density (calculated) 6.12 $Mg\ m^{-3}$

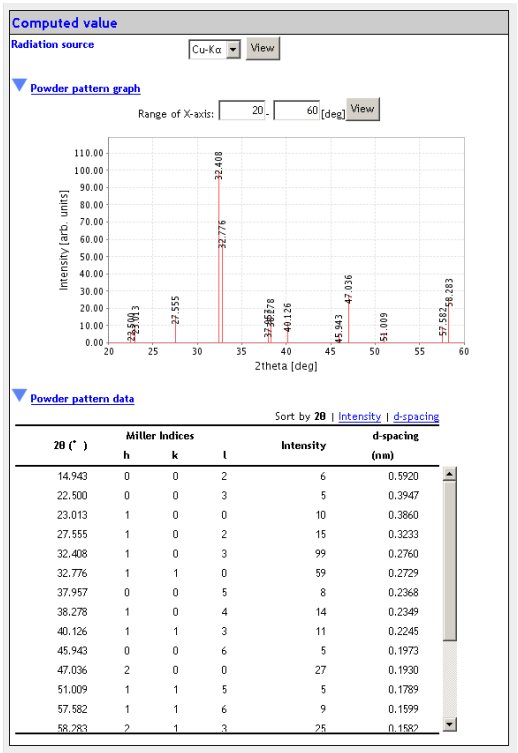
Z 1

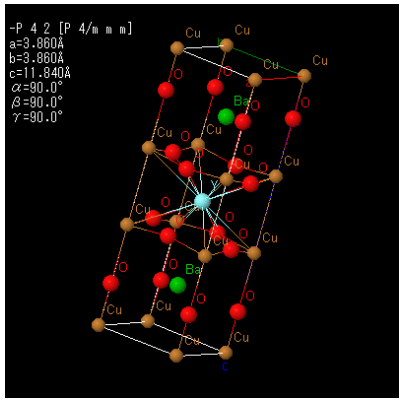
Atom coordinates

No	Site notation	Atom	Multiplicity	Wyckoff	Site symmetry	x	y	z	Occupancy
1	O1	O	4	i	2mm.	0	1/2	0.3792	1.0
2	Ba1	Ba	2	h	4mm	1/2	1/2	0.19522	1.0
3	O2	O	2	g	4mm	0	0	0.1522	1.0
4	Cu1	Cu	2	g	4mm	0	0	0.36103	1.0
5	Y1	Y	1	d	4/mmm	1/2	1/2	1/2	1.0
6	Cu2	Cu	1	a	4/mmm	0	0	0	1.0

Transition from Published Data to Standardized Data

Transition : No data.





Crystal structure and X-ray Diffraction

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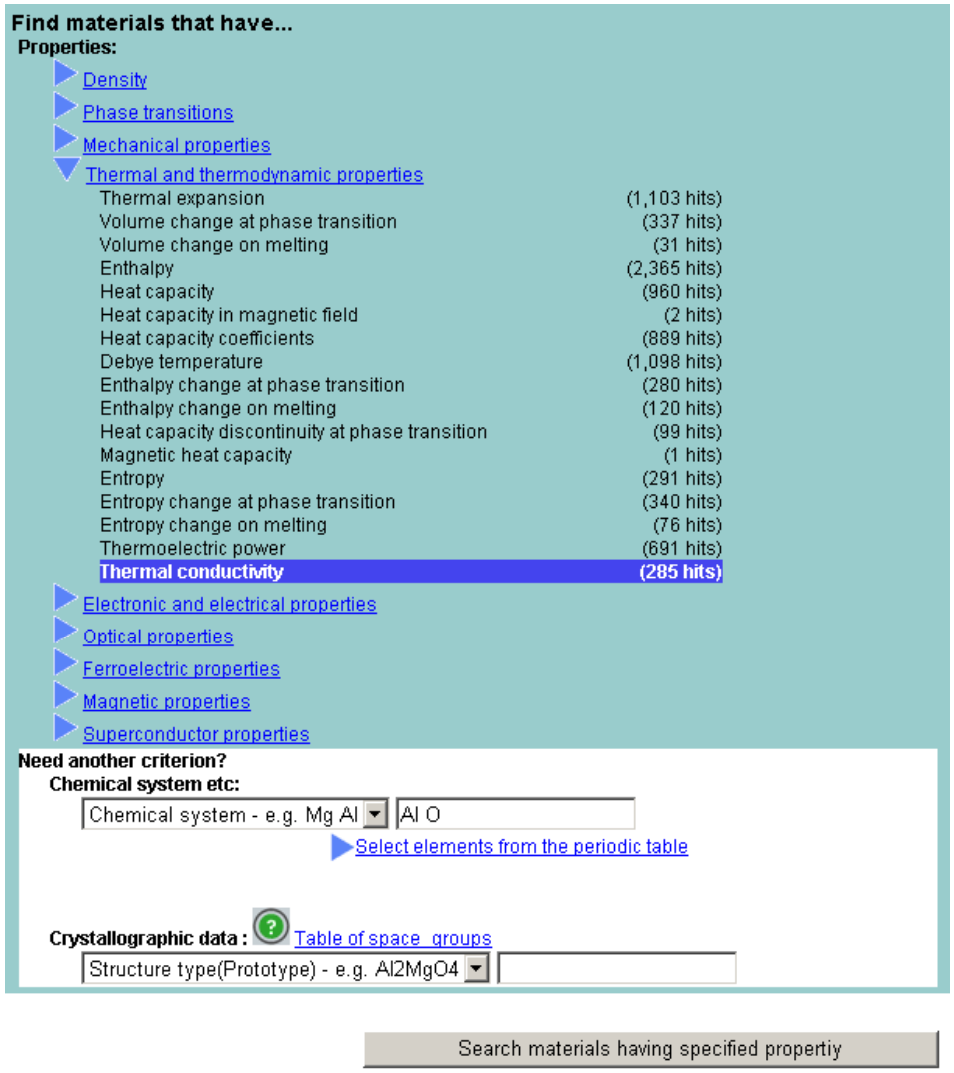
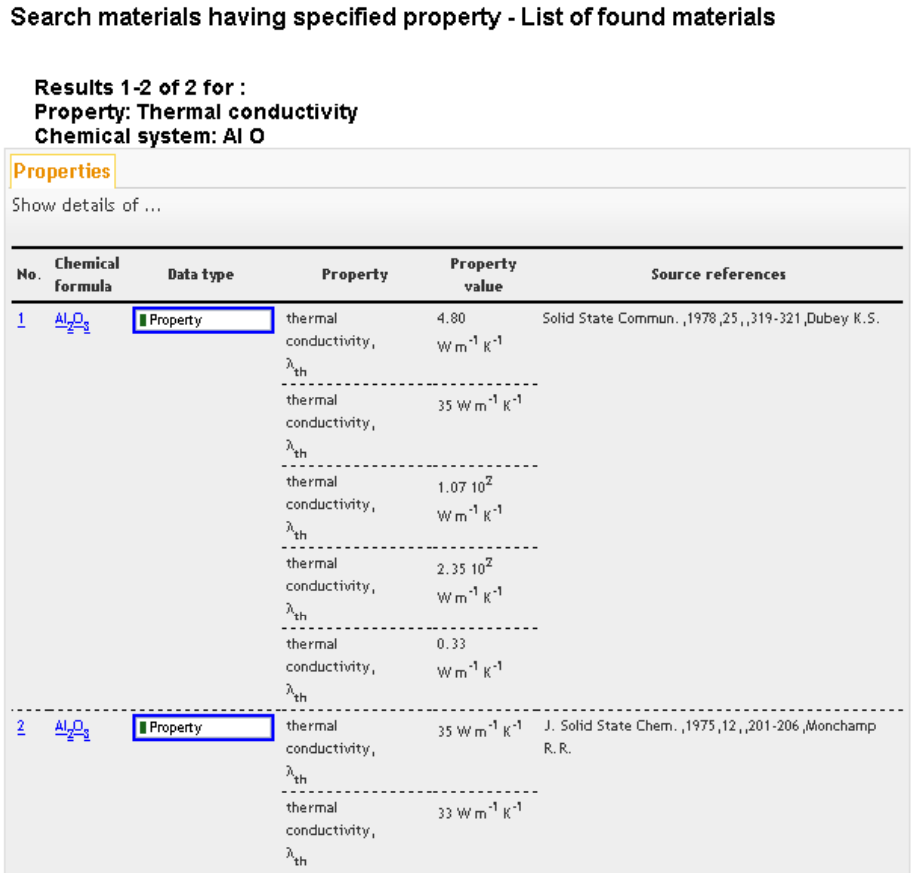


Property Search



Results of property search

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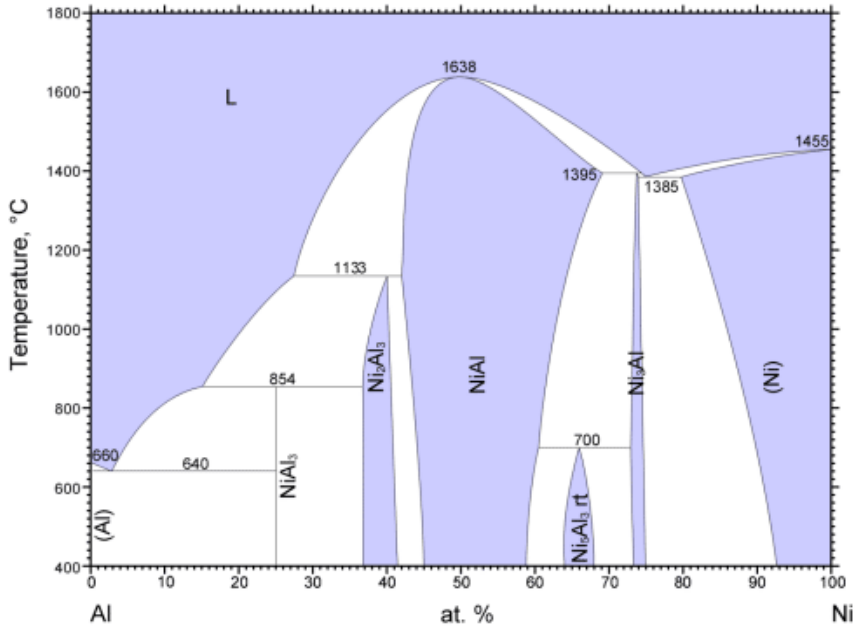

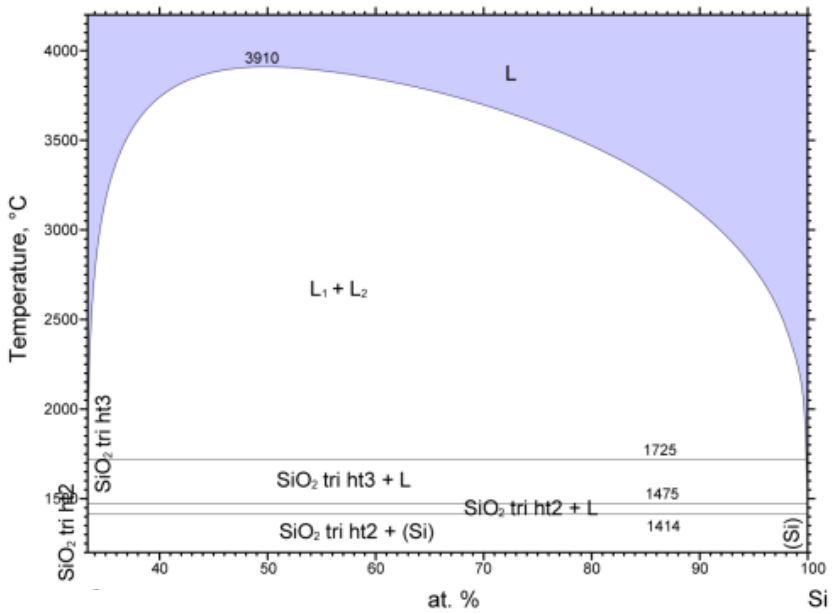

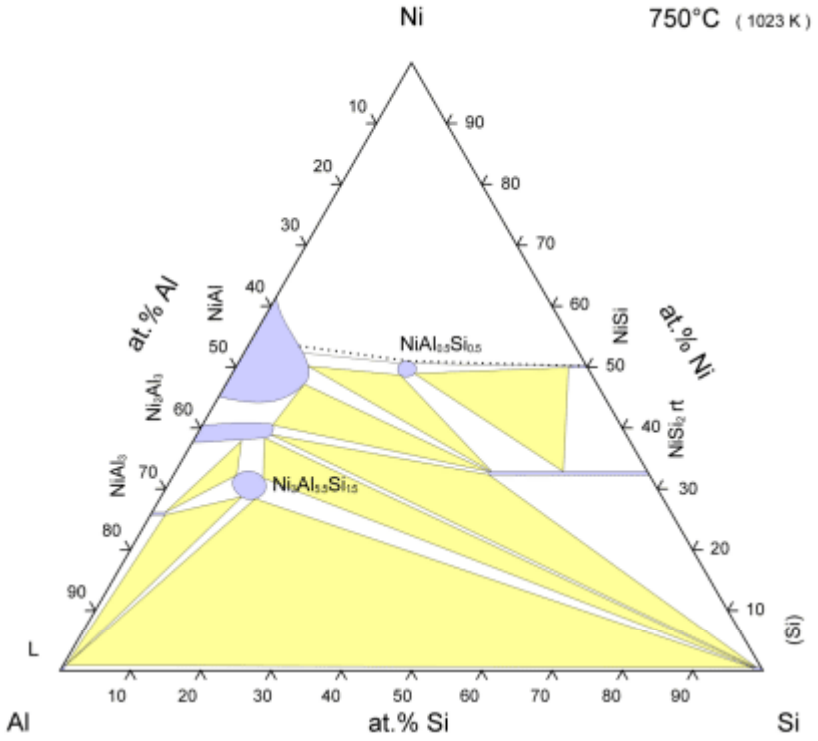

Binary and ternary phase diagrams

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Table Database products of inorganic materials

Products	Data contents	Publisher
ASM Alloy Phase Diagram Center	Phase Diagram	ASM International (USA)
ACerS-NIST Phase Equilibria Diagrams Database	Phase Diagram	American Ceramics Society, National Institute of Standards and Technology (USA)
ICSD Inorganic Crystal Structure Database	Crystal Structure	FIZ Karlsruhe (Germany), National Institute of Standards and Technology (USA)
ICDD PDF-4	Crystal Structure	International Centre for Diffraction Data (USA)
Pearson's Crystal Data	Crystal Structure	ASM International (USA)
CRYSTMET	Crystal Structure	Toth Information Systems, Inc. (Canada)
Pauling File Binary Edition	Binary phase diagram Crystal structure property	ASM International (USA)

Interfacial Thermal Conductance Database (ITC)

itc Interfacial thermal conductance database

To evaluate the interfacial thermal resistance, we have developed a program to calculate the interfacial thermal resistance using the crystal structures, Young's modulus, and the velocity of sound of the materials on the two sides of the interface, based on a diffusion mismatch model which has been established on the basis of mechanism of phonon diffuse scattering at the interface.

This database includes the thermal resistances of approximately 1000 interfaces, calculated using the diffusion mismatch model and measured by experiments.

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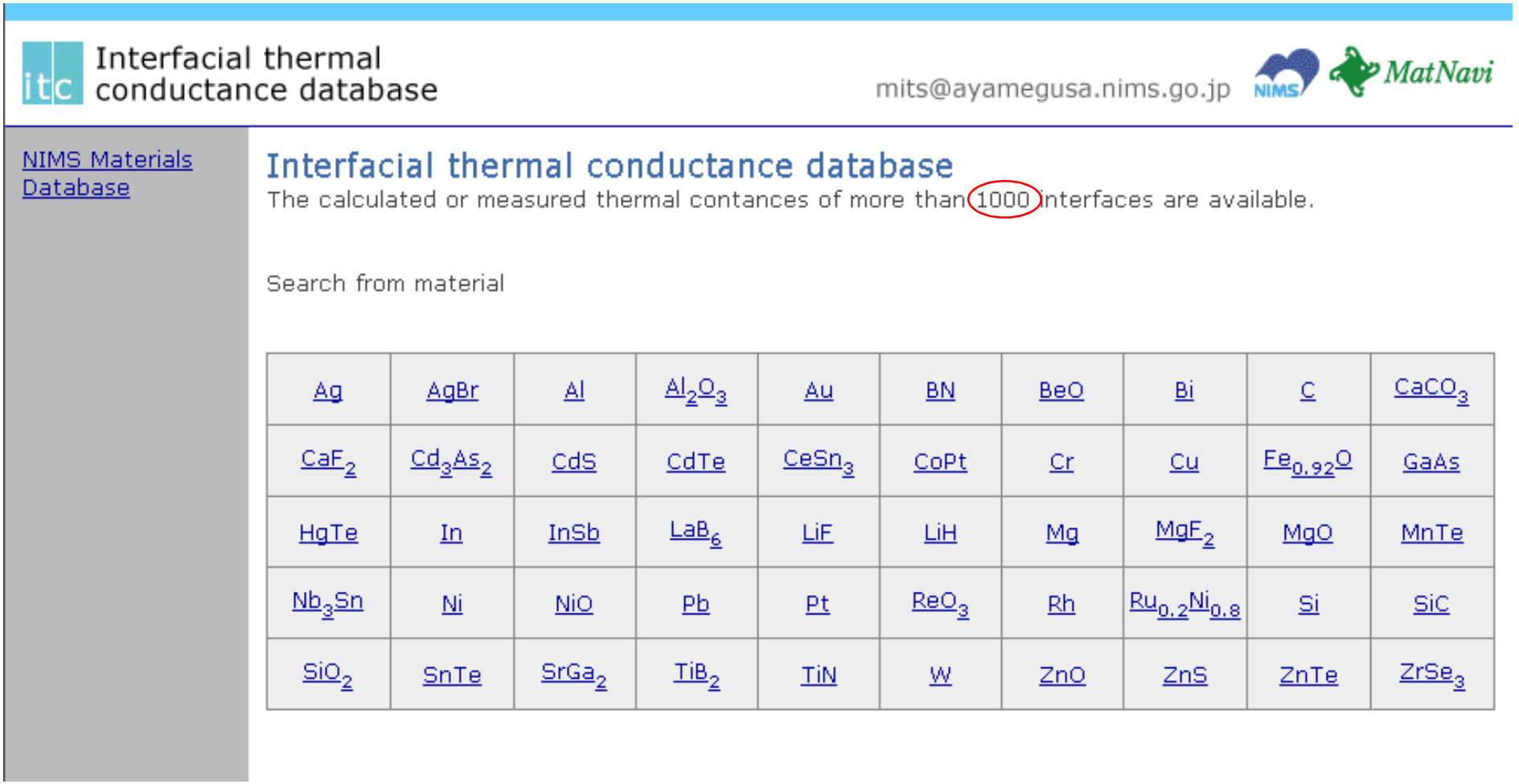

Search from material

Search from interfacial thermal conductance and Debye temperature ratio

Knowledge vase

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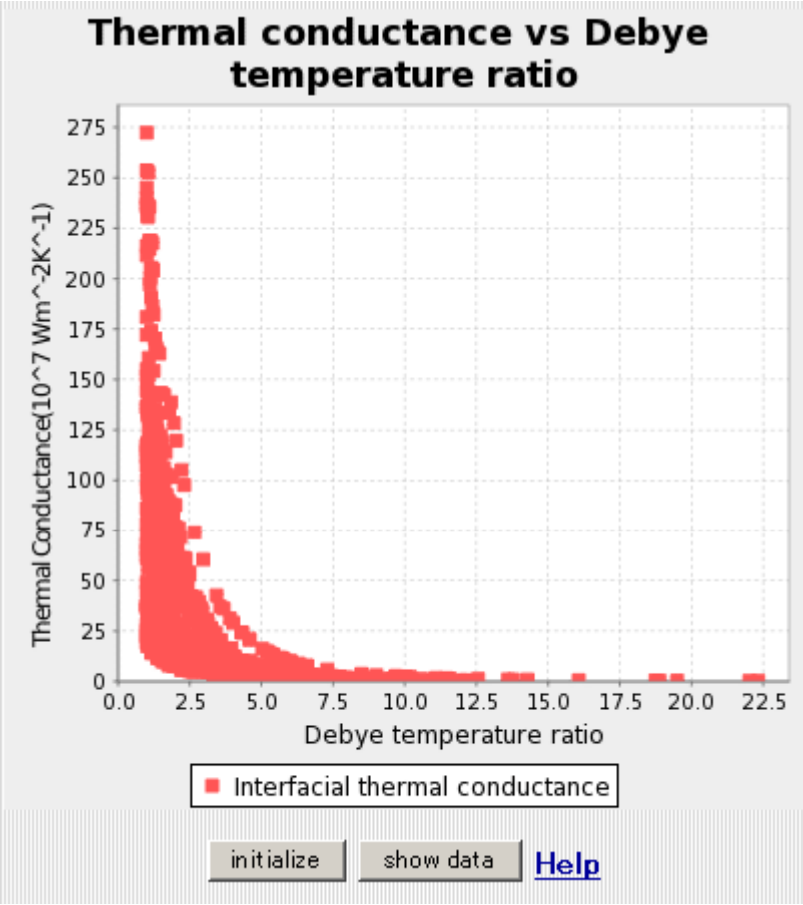

Search from the value of interfacial thermal conductance

Interfacial thermal conductance database

Al_2O_3-Au

Material 1 : Al_2O_3
Material 2 : Au
Composition Type : interface

Property

1.Physical Properties, Thermal Properties, Thermal Conductance

temperature(K),	thermal conductance($Wm^{-2}K^{-1}$)
300	34038613.4

Data obtaining method type : calculation
Data obtaining method : diffusion mismatch model

References

Haitao Wang, Yibin Xu, Masato Shimono, Yoshihisa Tanaka, Masayoshi Yamazaki : Computation of Interfacial Thermal Resistance by Phonon Diffuse Mismatch Model, (2007), in English, literature

Interfacial thermal conductance

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Computational Electronic Structure Database (CompES)

Electronic structures:	163
Reference data:	532
Element properties:	43
Crystal structures:	180

It comprises four components: The "Electronic Structures Database" contains the electronic structures of unary and binary materials obtained by first-principles calculations.

This main database is supplemented by three databases containing, respectively, the physical constants/properties of the elements and elemental solids, crystal structures, and reference data.

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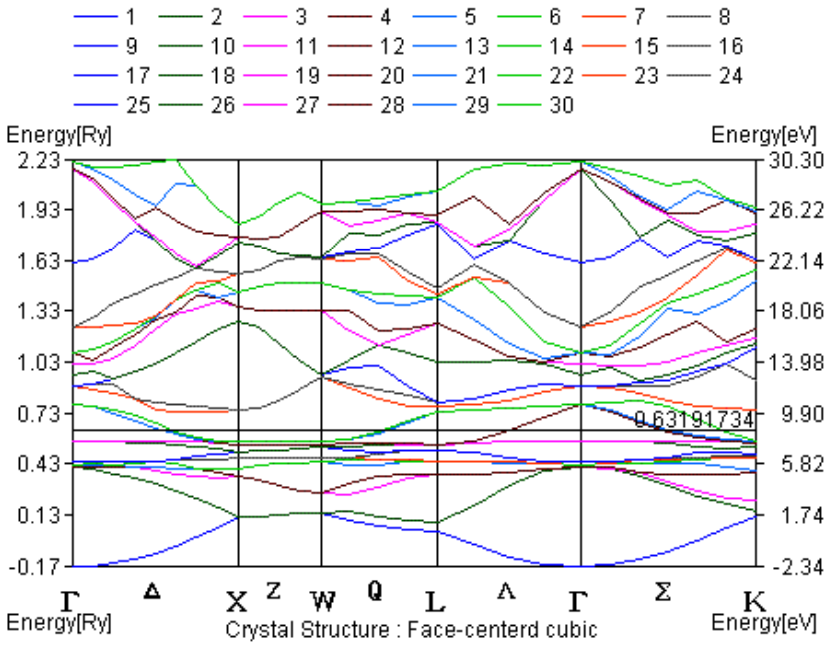
Band Structure

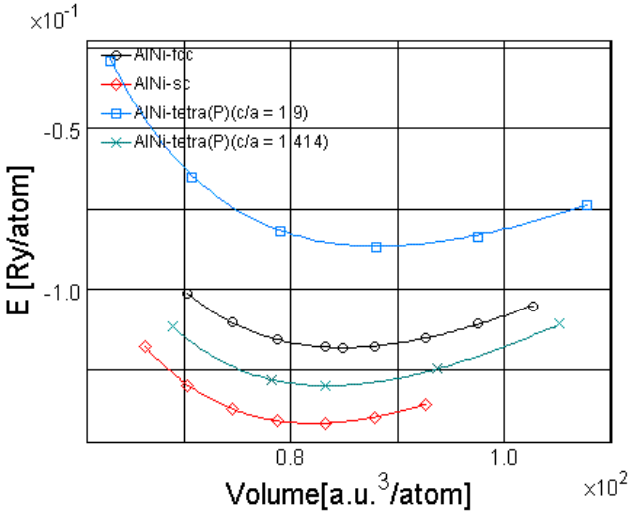
No.16 System: AlNi, NaTl(B32)/cF16, nm



Energy vs. wave number plot

Energy vs. volume

No.16 System: AlNi, NaTl(B32)/cF16, nm



B_0	0.00963
B'_0	4.2
v_0	84.85
$E(v_0)$	-0.11869
chi-square	1.9622e-08
R	0.99997
CONST	-1764.
$E_{tot} = E + CONST$	

Murnaghan's equation

$$E(v) = \frac{Bo \cdot v}{B'o \cdot (B'o - 1)} \left[B'o \cdot \left(1 - \frac{vo}{v}\right) + \left(\frac{vo}{v}\right)^{B'o} - 1 \right] + E(vo)$$

Total energy vs. volume plot

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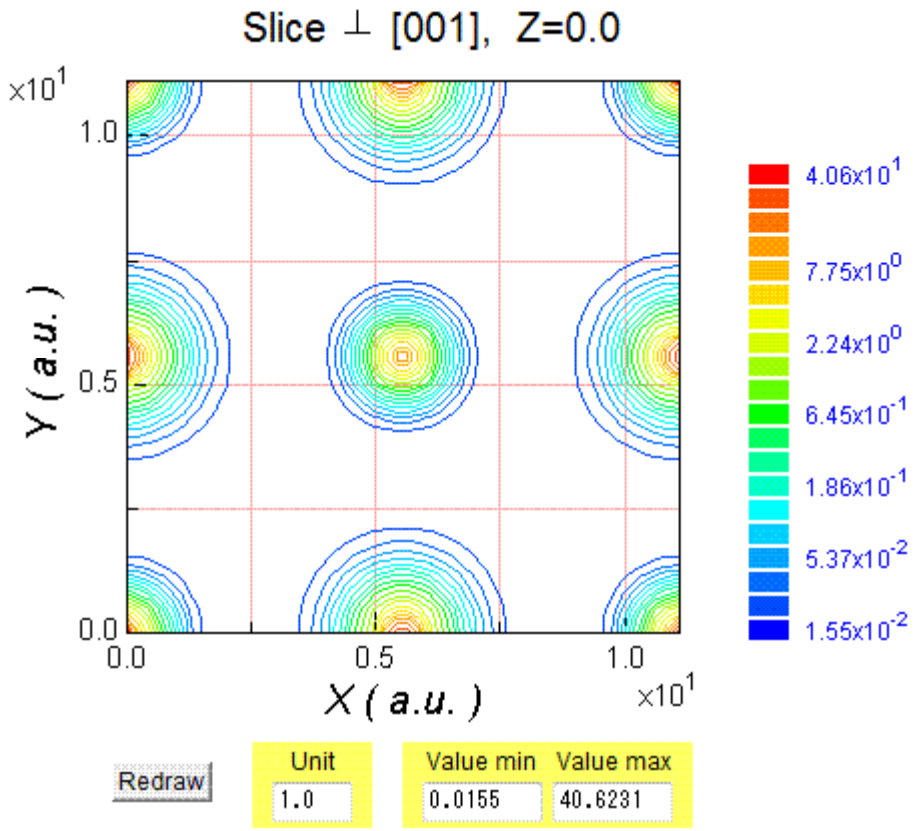
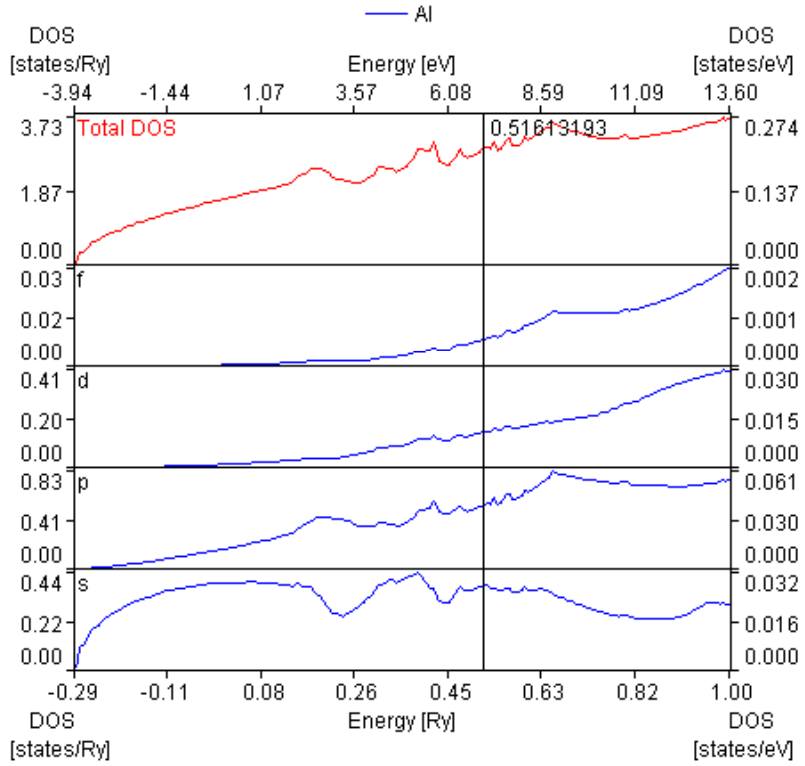
Total Charge Density (au^{-3})

No.16 System: AlNi, NaTl(B32)/cF16, nm



Density of States

No.4 System: Al, W(A2)/cI2, nm



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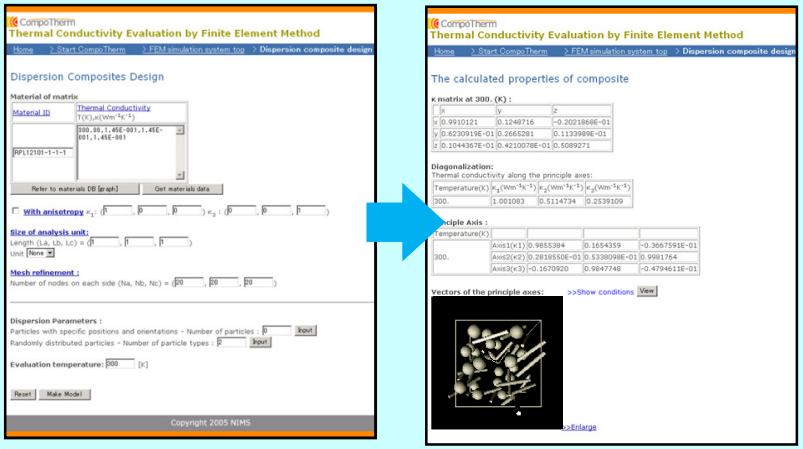
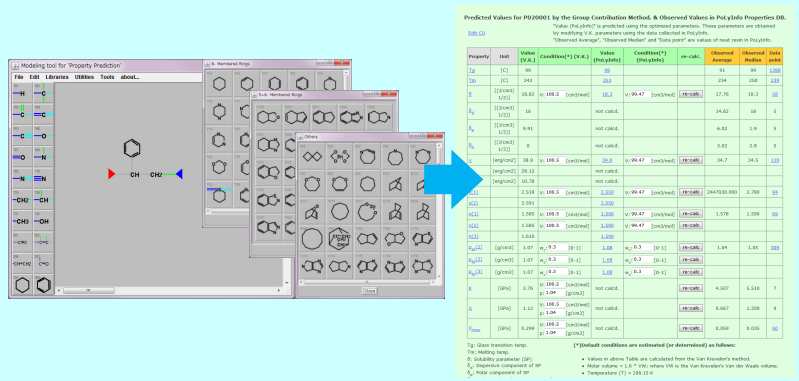
No.	Application System
1	**Composite Design & Property Prediction System (CompoTherm)**
2	**Polymer Properties Prediction System**
3	**Metal Segregation Prediction System (SurfSeg)**
4	**Weld Thermal History Simulator**

Application of MatNavi



Composite Design & Property Prediction System (CompoTherm)



Polymer Properties Prediction System

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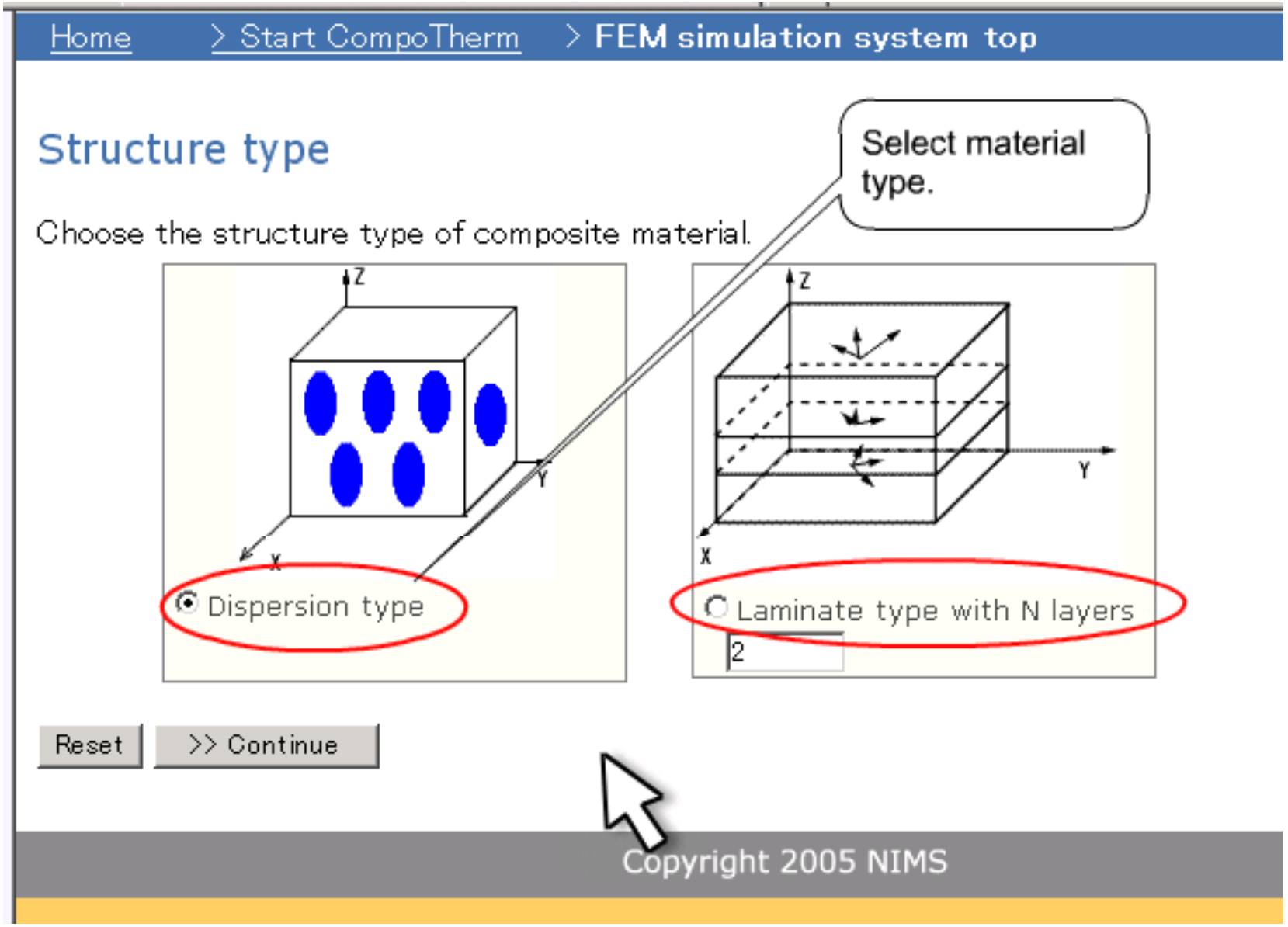
Composite Design & Property Prediction System (CompoTherm)

CompoTherm

- CompoTherm is an integrated platform which can help you design a composite material with required thermophysical properties. The main functions provided by CompoTherm include: Material selection, Composite structure design
- Thermophysical property (thermal conductivity, thermal diffusivity, specific heat, etc.) prediction
- Knowledge base about composite and thermophysical properties Database of interfacial thermal conductance.

Calculate the density, specic heat, thermal conductivity and thermal diusivity of the designed composites using the law of mixture, equivalent inclusion method and effective medium theory, etc. Easy modeling and quick calculation, suitable for investigating the dependence of thermo-physical properties on structure.
Thermo-physical property data of polymers, alloys and ceramics extracted from NIMS Materials Databases are available.



Demonstration of the finite element analysis system screen on CompoTherm

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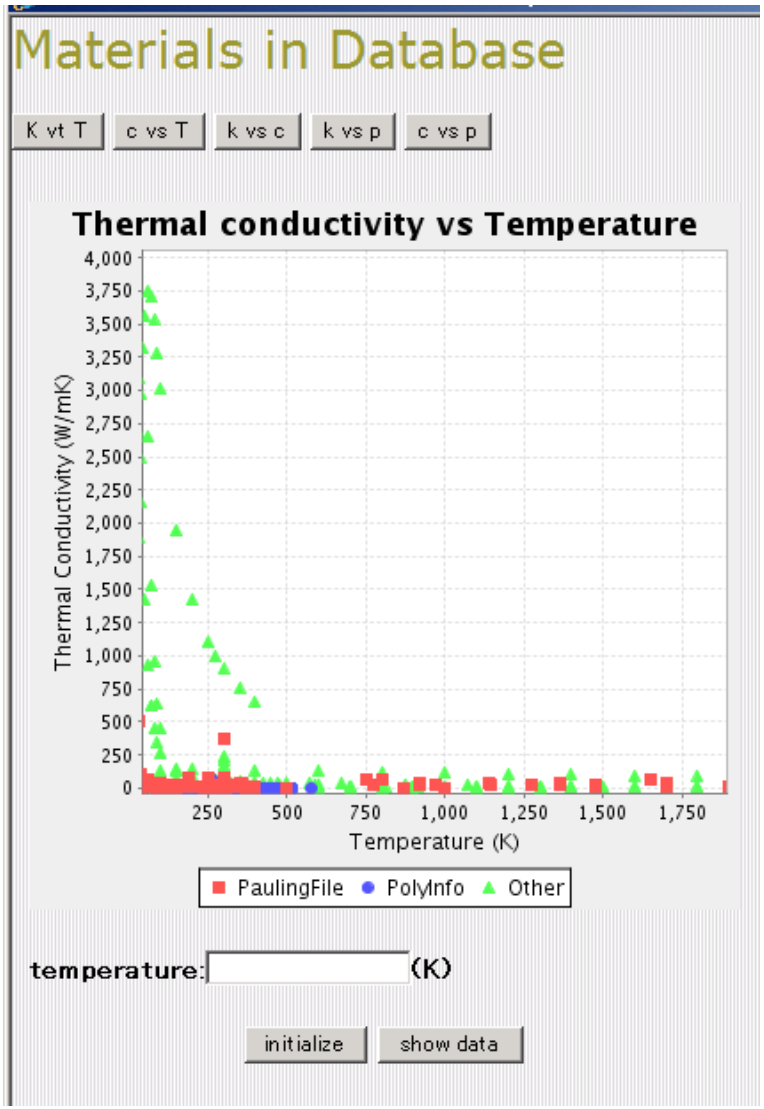

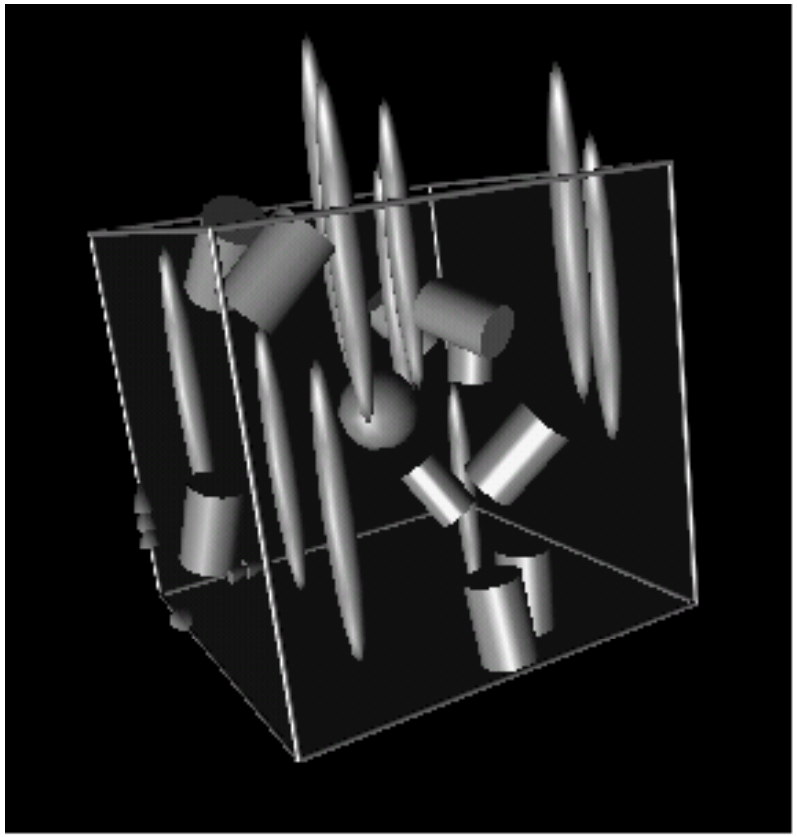

3D model of a composite material case created by CompoTherm

Plot of the thermal conductivity of the thermal properties database

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Metal Segregation Prediction System (SurfSeg)

SurfSeg

- Prediction of surface segregation between two annealed metals

SurfSeg is designed to simulate surface or interface segregation in the following four cases (at the time of April 2009, only the first one is available). Materials are approximated as a uniform media, therefore, the crystal orientation dependence of physical properties relating to the segregation is not taken into account for the simulation.

surface segregation in film/substrate system (available from April 2009)
surface segregation in dilute alloy system (available in the future)
interface segregation at film-substrate interface (available in the future)
interface segregation at alloy-substrate interface (available in the future)

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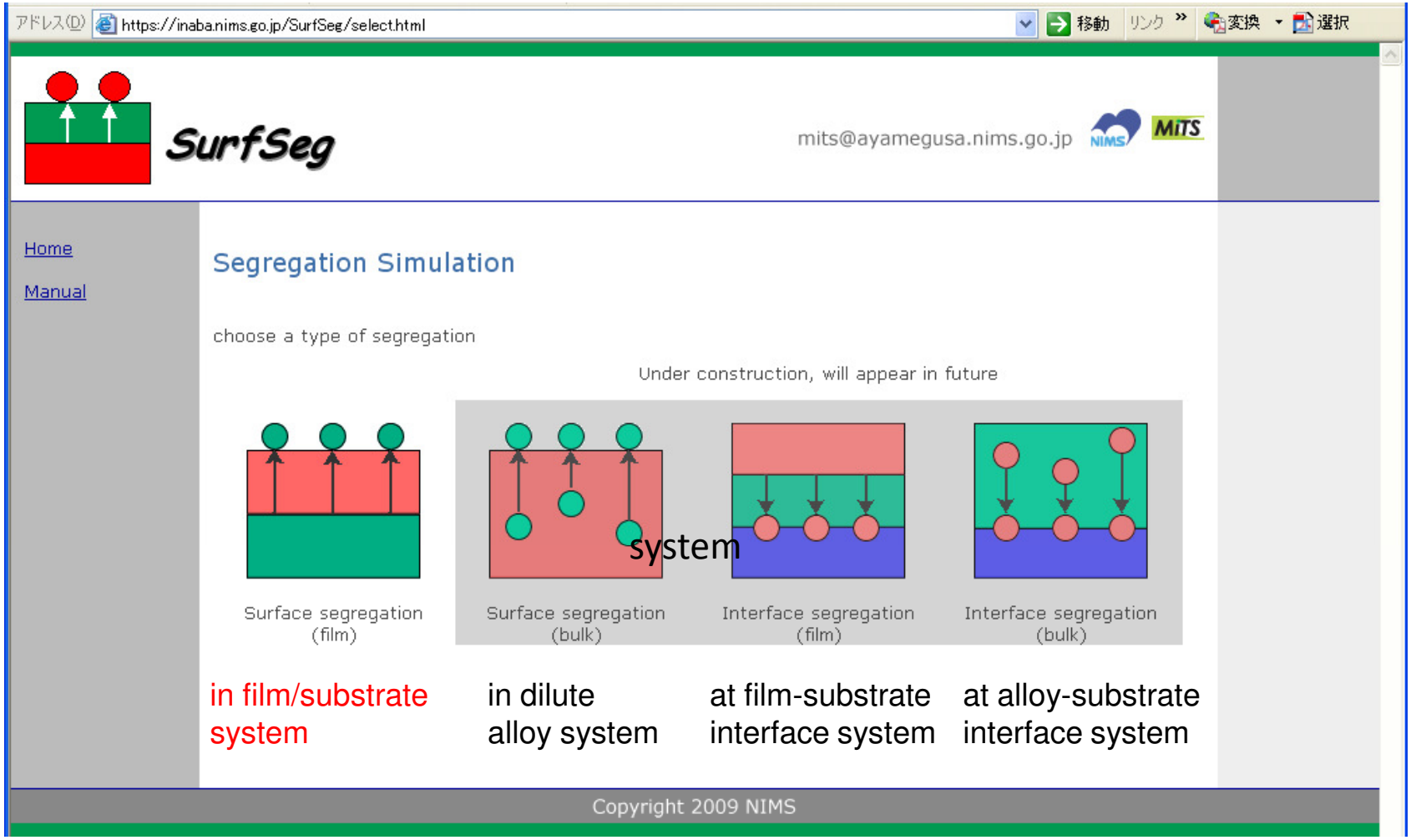
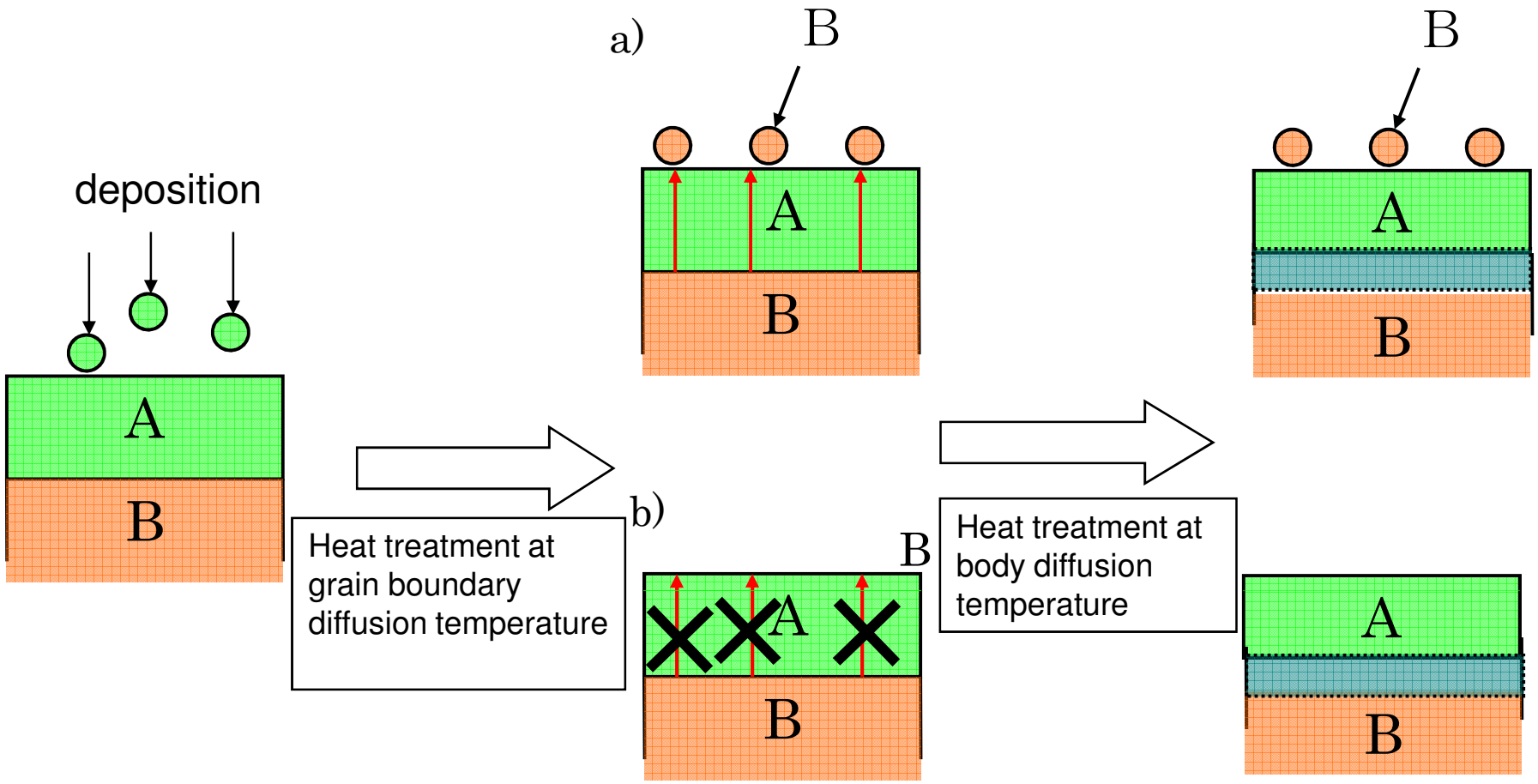


The first screen of the metal segregation prediction system SurfSeg.



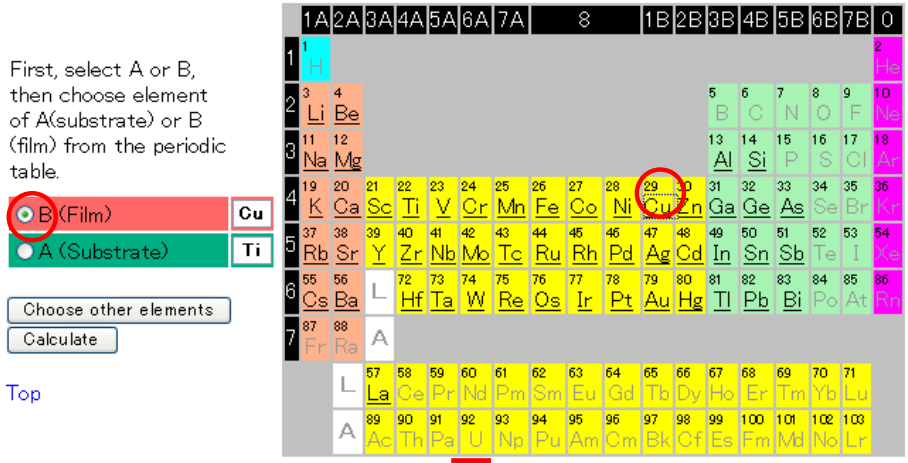
Schematic diagram of a metal laminate film segregation in this system

What can you use SurfSeg for ?

Help in selecting materials for surface property modification, while preserving the initial bulk properties such as mechanical strength and electrical conductivity. For example:

1. Anti-corrosion, adhesion, antibacterial or catalytic reactions, work function & Schottky barrier control, etc. i.e. fnding a system which shows segregation of a desirable element.
2. Diusion barrier: finding B that does not let A segregate on the surface. If A segregates on B, B is not suitable for difusion barrier.

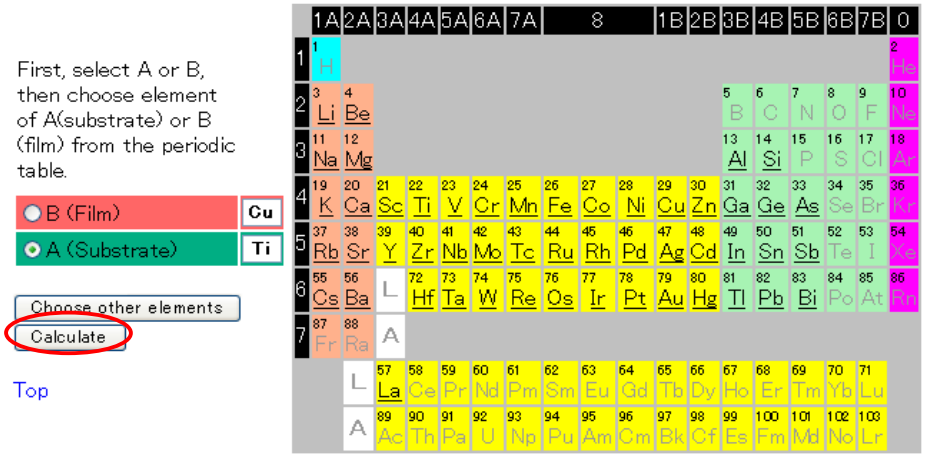
Select elements of each film and base from periodic table



Available for combinations of 51 elements x 51 elements

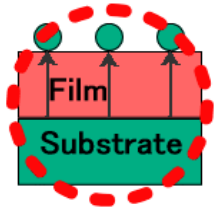
Input screen

Click ‘Calculate’ and then results are shown



predicted results

Adsorption energy
Ti on Cu : 371 kJ/mol
Ti on Ti : 363 kJ/mol



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Summary

- The largest advantage of a database is the possibility of re-organizing and transforming its contents to any other formats, and the easiness of integrating with other computer systems.
- Materials database development is a long-term challengeable task. A self-supporting mechanism must be established.
- Global collaboration of sharing and integrating the existing data resources is a solution for making efficient use and enhancing the value of each database.

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

Ogata.toshio@nims.go.jp

The base of COMPUTER NETWORK is HUMAN NETWORK

MatNavi

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Thank you for your attention.