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New stage of MatNavi, materials database at NIMS

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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**

New 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

Free of Charge

MatNavi is one of the world's largest materials databases of polymer, ceramic, alloy, superconducting material, composite and diffusion.

MatNavi
NIMS Materials Database

Japanese For New User National Institute for Materials Science, Materials Information Station

Home About us MITS Symposium Link Contact us NIMS

"MatNavi" is one of the world's largest materials databases provided by NIMS

Database

- Basic Properties
 - Polymer Database (PolVinfo)
 - Inorganic Material Database (AtomWork)
 - Computational Electronic Structure Database (CompES)
 - Database of Promising Adsorbents for Decontamination of Radioactive Substances (READS)
 - Neutron Transmutation Database (NeuTran)
 - Interfacial Thermal Conductance Database (ITC)
 - Diffusion Database (Kakusan)
 - Superconducting Material Database (SuperCon)
- NIMS Structural Materials Data Sheet Online
 - Creep Data Sheet (CDS)
 - Fatigue Data Sheet (FDS)
 - Corrosion Data Sheet (CoDS)
 - Space Use Materials Strength Data Sheet (SDS)
 - Metallic Material Microstructure Database (Kinsu)
- Engineering
 - Metallic Material Database (Kinzoku)
 - CCT Diagram Database (CCTD)
 - Materials Risk Information Platform (MRIP)
- Applications
 - Composite Design & Property Prediction System (CompoTherm)
 - Polymer Properties Prediction System
 - Metal Segregation Prediction System (SurfSeg)
 - Weld Thermal History Simulator

Users

New Users:
The use of "MatNavi" is free. (Free of charge)
All you need to do is register.
[Register](#)

Registered Users:
Please select a database and login from the "Enter" on each page. E-mail address and password are necessary.
[Forgot your Password ?](#)
[Update registration](#)
[Close your account](#)

MatNavi Search

MatNavi Search

Keyword Search

AND OR Contain

Tree Search

- Material
 - Element
 - Alloy
 - Ceramic
 - Polymer
- Property
 - Crystal Structure
 - Micrograph
 - Phase Transition
 - Mechanical Properties
 - Physical Properties
 - Physicochemical Property
 - Chemical Properties

Materials information from NIMS

- National Institute for Materials Science (NIMS)
- Nanotech Japan
- Materials Science Outlook
- SANZEN - electronic structure software
- NIMS Thermodynamic Database

Partners

- Matdata.net (Granta Design)
- MatWeb (Automation Creations Inc.)
- Springer Link (Landolt Bornstein)
- LB Substance / Property Index
- Materials Bank (Korea)
- "Crystal" Database (Russia)
- RIQ-DB (AIST)

News

[Aug. 01, 2012] [Metal Segregation Prediction System \(SurfSeg\)](#) prediction under oxygen atmosphere is now available.

[Jun. 12, 2012] [Creep Data Sheet](#) No.48A, 49A were added.
[Fatigue Data Sheet](#) No.116, 117 were added.

Notes on Use

- [System Requirements \(Plug-ins\)](#)
- [Site policy](#)
- [Leaflet download](#)
- [Feedback](#)

Registered users: 70,676
Countries: 141, Organizations: 18,121

NIMS Materials Database (MatNavi) will be unavailable due to system maintenance from 5:00 PM to 6:00 PM (GMT+9) every Wednesday.

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Registration

Search engine

Information

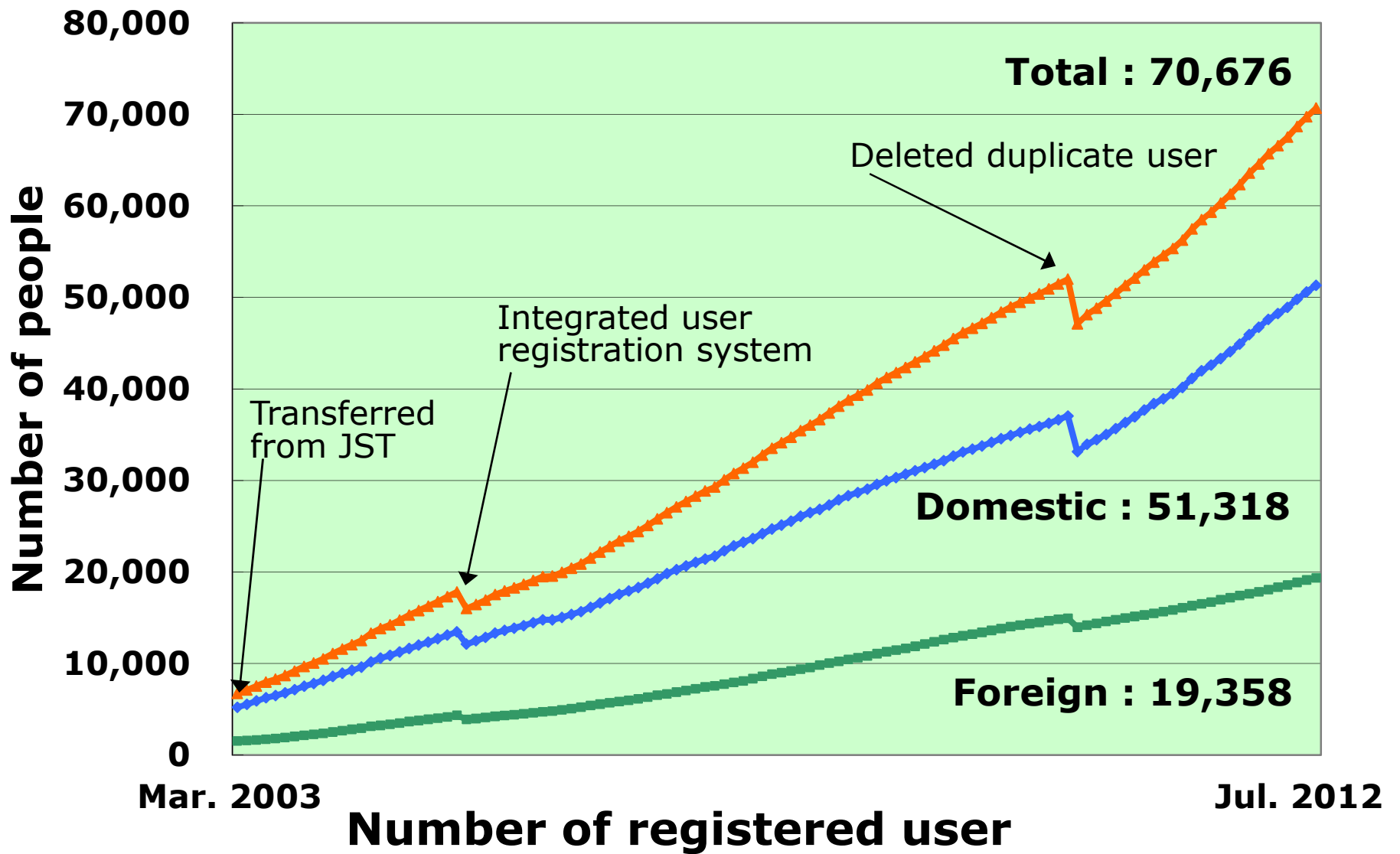
Links with external organizations

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



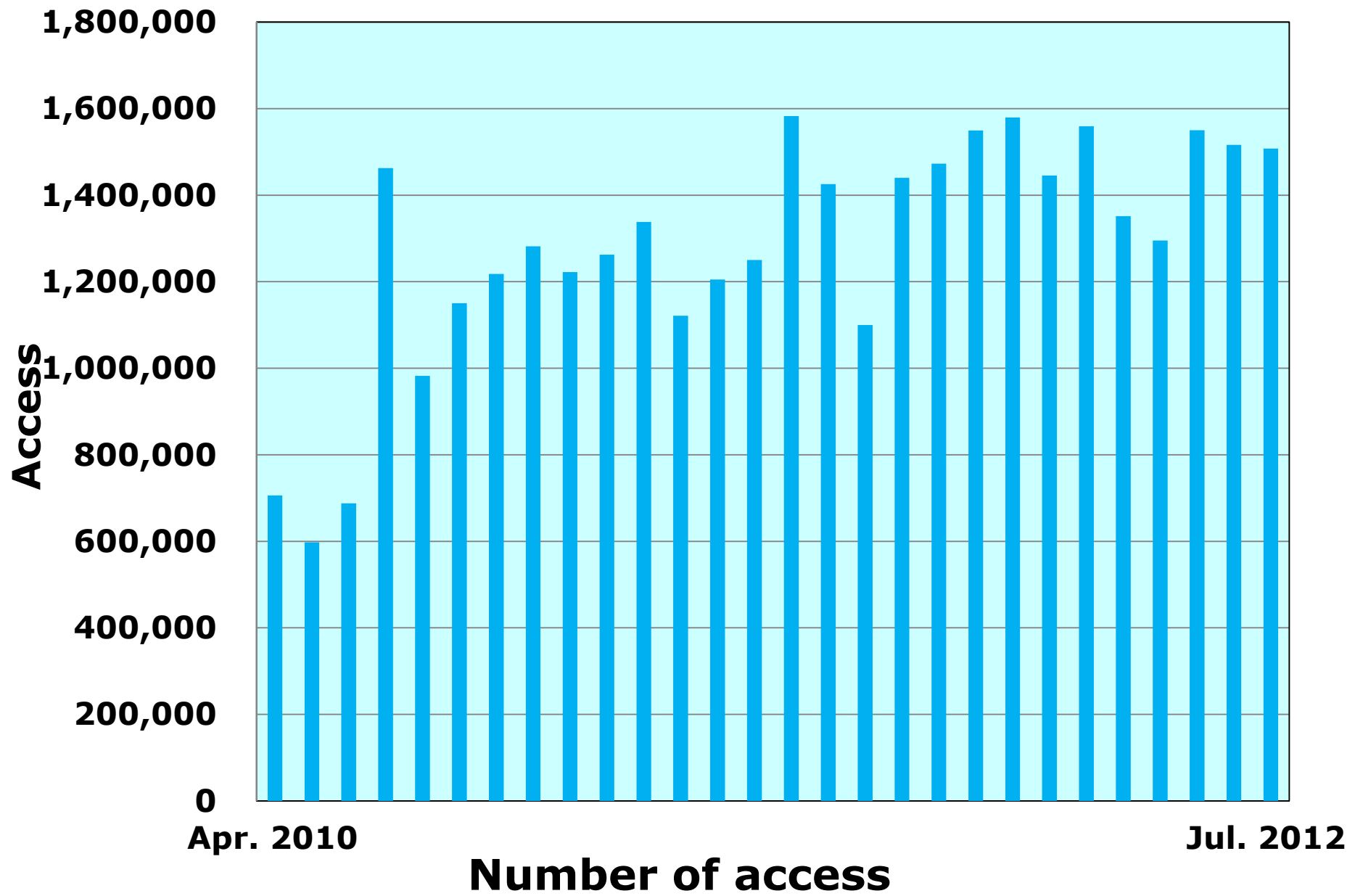
No.	Database System	Data Source	
		Experimental or Calculation	Literature
1	Polymer Database (PoLyInfo)		○
2	Inorganic Database (AtomWork)		○
3	Computational Electronic Structure Database (CompES)	○	
4	Database of Promising Adsorbents for Decontamination of Radioactive Substance (READS)	○	
5	Neutron 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



Registered users: 70,676 (Domestic: **51,318**, Foreign: **19,358**)

Locations: 141, Organizations: 18,121 (at Jul. 31, 2012)



Inorganic Database (AtomWork)



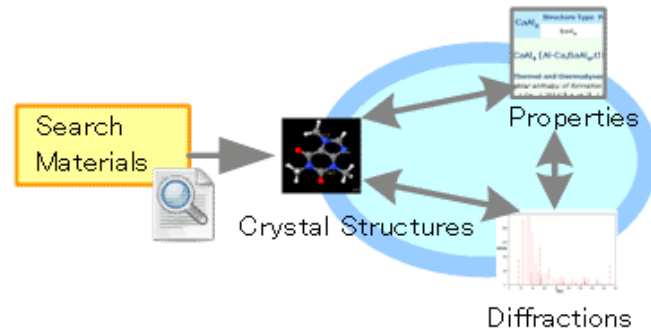
The Inorganic Material Database aims to cover all **basic crystal structure, x-ray diffraction, property and phase diagram data** of inorganic and metallic materials from main literature sources.

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.**

Search materials - Setting for search conditions



Selection Search system

Find materials that have...

Chemical system - e.g. Mg Al

[Select elements from the periodic table \(for Chemical system\)](#)

1																	18
1 H	2 He											13 B	14 C	15 N	16 O	17 F	18 Ne
3 Li	4 Be											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
11 Na	12 Mg	3	4	5	6	7	8	9	10	11 Cu	12 Zn	13 Ga	14 Ge	15 As	16 Se	17 Br	18 Kr
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra	89 Ac	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Nh	114 Fl	115 Mc	116 Lv	117 Ts	118 Og
Lanthanoids (Ln)		57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu	
Actinoids (An)		89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr	

Need another criterion? (crystallographic data, etc.) [Table of space groups](#)

Structure type(Prototype) - e.g. Al2MgO4

Material Search

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,

$\alpha = 90^\circ$, $\beta = 90^\circ$, $\gamma = 90^\circ$

Cell volume 0.17641 nm³

Crystal Structure (Standardized)

Crystallographic data

Cell parameters a = 0.386 nm, b = 0.386 nm, c = 1.184 nm,

$\alpha = 90^\circ$, $\beta = 90^\circ$, $\gamma = 90^\circ$

Cell volume 0.1764 nm³

Cell density (calculated) 6.12 Mg m⁻³

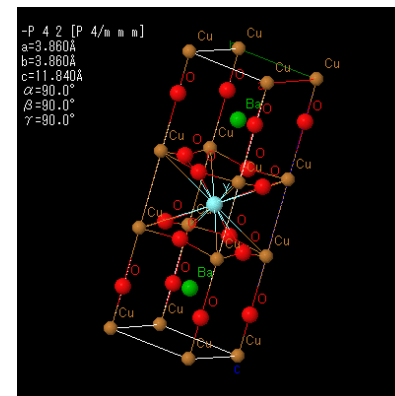
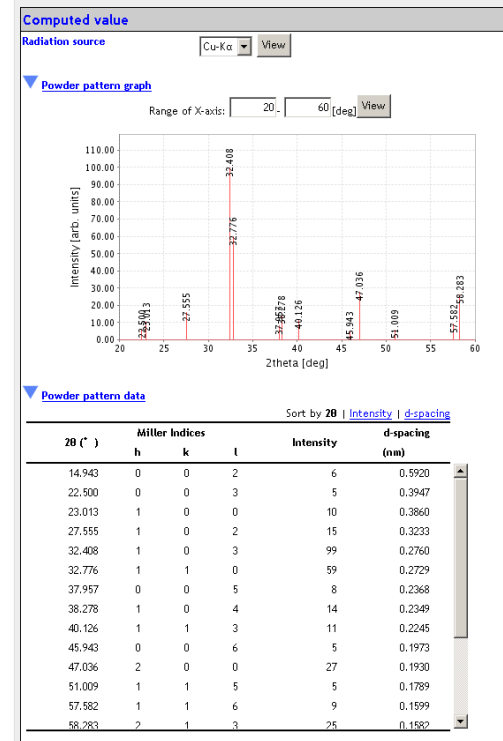
Z 1

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

Find materials that have...

Properties:

- [Density](#)
- [Phase transitions](#)
- [Mechanical properties](#)
- [Thermal and thermodynamic properties](#)

Thermal expansion	(1,103 hits)
Volume change at phase transition	(337 hits)
Volume change on melting	(31 hits)
Enthalpy	(2,365 hits)
Heat capacity	(960 hits)
Heat capacity in magnetic field	(2 hits)
Heat capacity coefficients	(889 hits)
Debye temperature	(1,098 hits)
Enthalpy change at phase transition	(280 hits)
Enthalpy change on melting	(120 hits)
Heat capacity discontinuity at phase transition	(99 hits)
Magnetic heat capacity	(1 hits)
Entropy	(291 hits)
Entropy change at phase transition	(340 hits)
Entropy change on melting	(76 hits)
Thermoelectric power	(691 hits)
Thermal conductivity	(285 hits)

- [Electronic and electrical properties](#)
- [Optical properties](#)
- [Ferroelectric properties](#)
- [Magnetic properties](#)
- [Superconductor properties](#)

Need another criterion?

Chemical system etc:

Chemical system - e.g. Mg Al

[Select elements from the periodic table](#)

Crystallographic data: [Table of space groups](#)

Structure type(Prototype) - e.g. Al₂MgO₄

Search materials having specified property

Property Search

Search materials having specified property - List of found materials

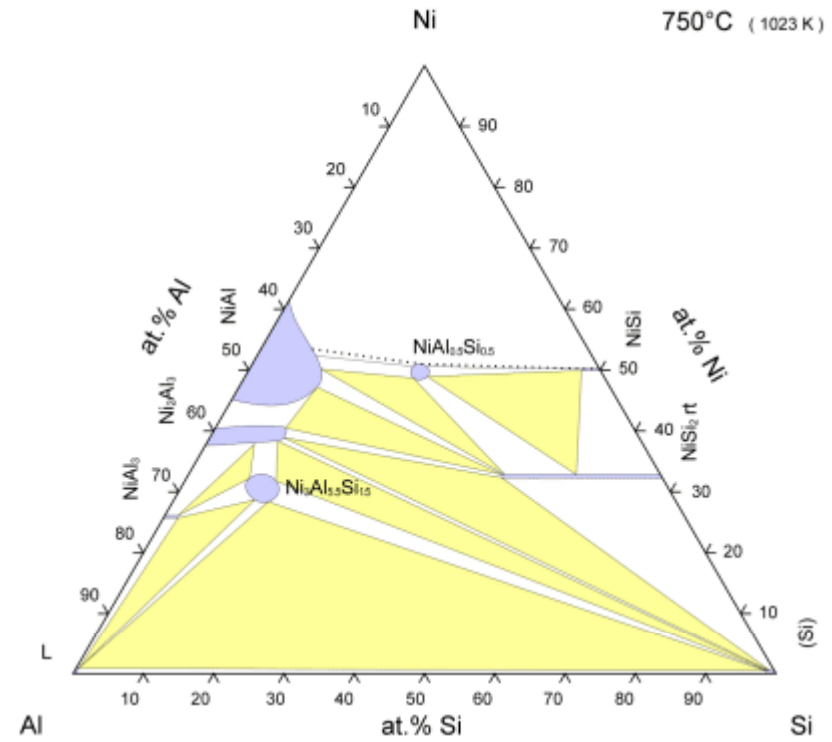
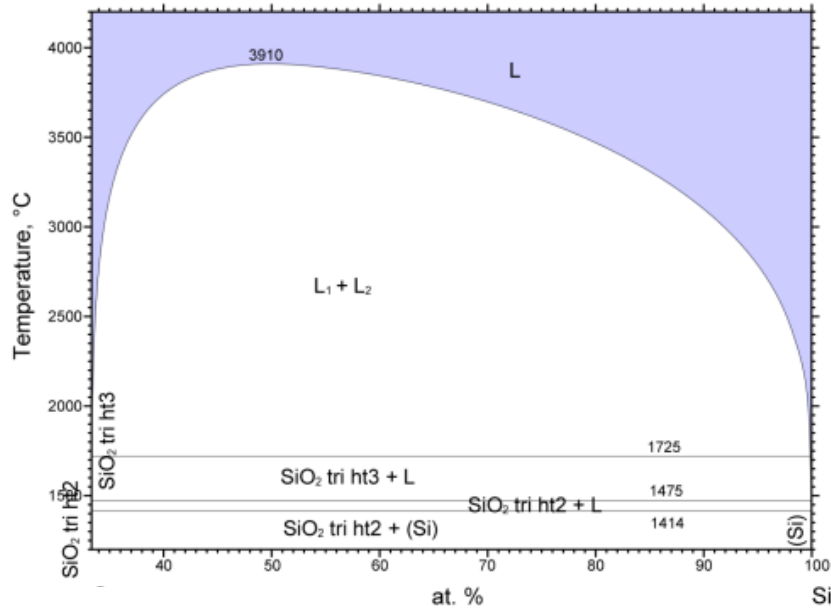
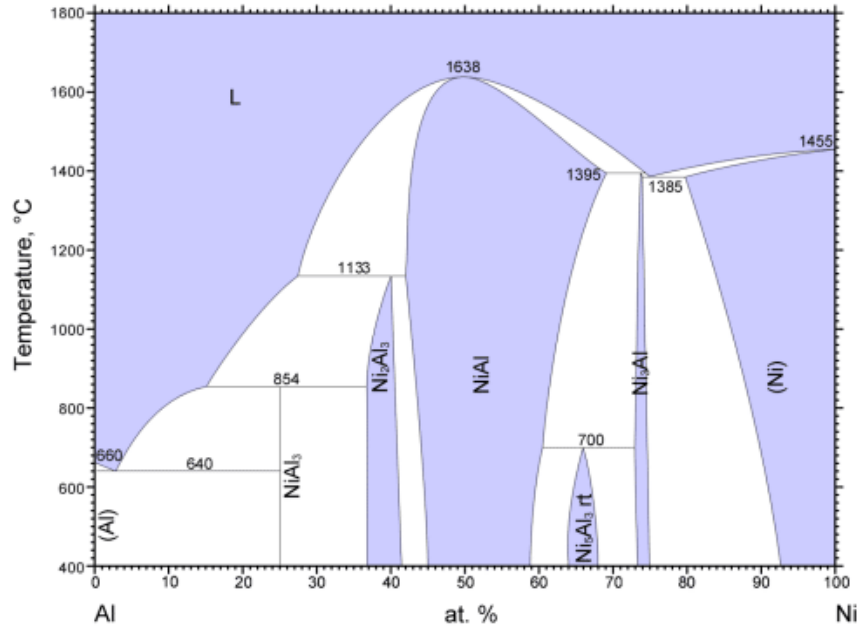
Results 1-2 of 2 for :
Property: Thermal conductivity
Chemical system: Al O

Properties

Show details of ...

No.	Chemical formula	Data type	Property	Property value	Source references
1	Al_2O_3	Property	thermal conductivity, λ_{th}	4.80 $\text{W m}^{-1} \text{K}^{-1}$	Solid State Commun. ,1978,25,,319-321,Dubey K.S.
			thermal conductivity, λ_{th}	35 $\text{W m}^{-1} \text{K}^{-1}$	
			thermal conductivity, λ_{th}	$1.07 \cdot 10^2 \text{ W m}^{-1} \text{K}^{-1}$	
			thermal conductivity, λ_{th}	$2.35 \cdot 10^2 \text{ W m}^{-1} \text{K}^{-1}$	
2	Al_2O_3	Property	thermal conductivity, λ_{th}	35 $\text{W m}^{-1} \text{K}^{-1}$	J. Solid State Chem. ,1975,12,,201-206,Monchamp R.R.
			thermal conductivity, λ_{th}	33 $\text{W m}^{-1} \text{K}^{-1}$	

Results of property search



Binary and ternary phase diagrams

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)



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.

Interfacial thermal conductance database

The calculated or measured thermal conductances of more than 1000 interfaces are available.

Search from material

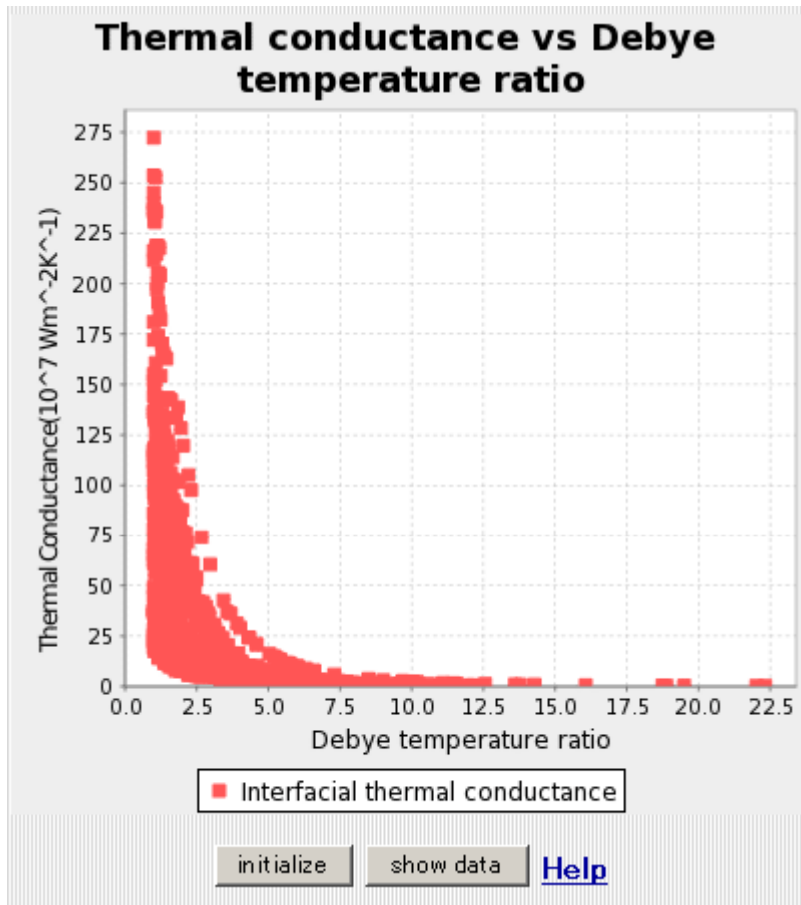
Ag	AgBr	Al	Al₂O₃	Au	BN	BeO	Bi	C	CaCO₃
CaF₂	Cd₃As₂	CdS	CdTe	CeSn₃	CoPt	Cr	Cu	Fe_{0.92}O	GaAs
HgTe	In	InSb	LaB₆	LiF	LiH	Mg	MgF₂	MgO	MnTe
Nb₃Sn	Ni	NiO	Pb	Pt	ReO₃	Rh	Ru_{0.2}Ni_{0.8}	Si	SiC
SiO₂	SnTe	SrGa₂	TiB₂	TiN	W	ZnO	ZnS	ZnTe	ZrSe₃

Search from material

[Search from interfacial thermal conductance and Debye temperature ratio](#)

[Knowledge base](#)

Interfacial thermal conductance database



$\text{Al}_2\text{O}_3\text{-Au}$

Material 1 : [Al₂O₃](#)

Material 2 : [Au](#)

Composition Type : interface

Property

1.Physical Properties, Thermal Properties, Thermal Conductance

temperature(K)	thermal conductance($\text{Wm}^{-2}\text{K}^{-1}$)
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

Search from the value of interfacial thermal conductance

Computational Electronic Structure Database (CompES)



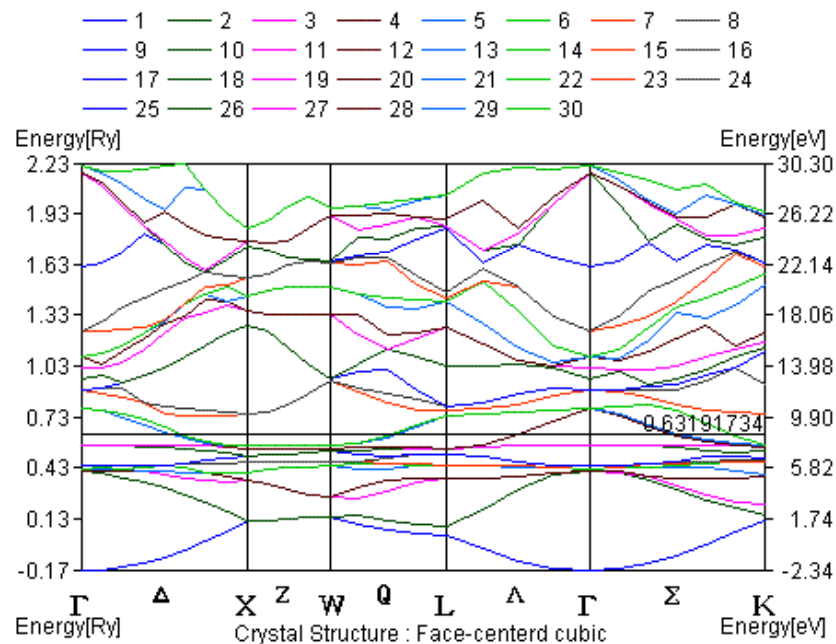
Electronic structures:	163
Reference data:	532
Element properties:	43
Crystal structures:	180

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.**

Band Structure

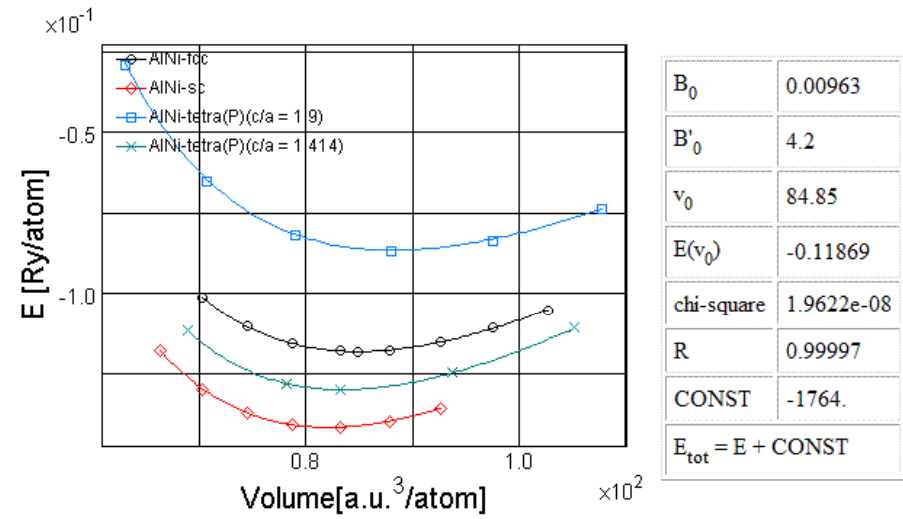
No.16 System: AlNi, NaTl(B32)/cF16, nm



Energy vs. wave number plot

Energy vs. volume

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



Murnaghan's equation

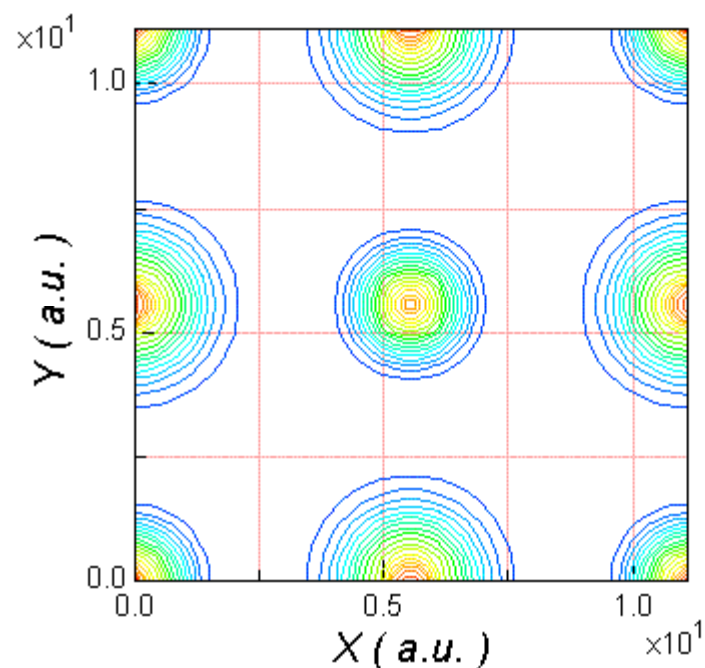
$$E(v) = \frac{B_0 \cdot v}{B_0 \cdot (B_0 - 1)} \left[B_0 \cdot \left(1 - \frac{v_0}{v}\right) + \left(\frac{v_0}{v}\right)^{B_0} - 1 \right] + E(v_0)$$

Total energy vs. volume plot

Total Charge Density (au^{-3})

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

Slice \perp [001], Z=0.0



Redraw

Unit

1.0

Value min

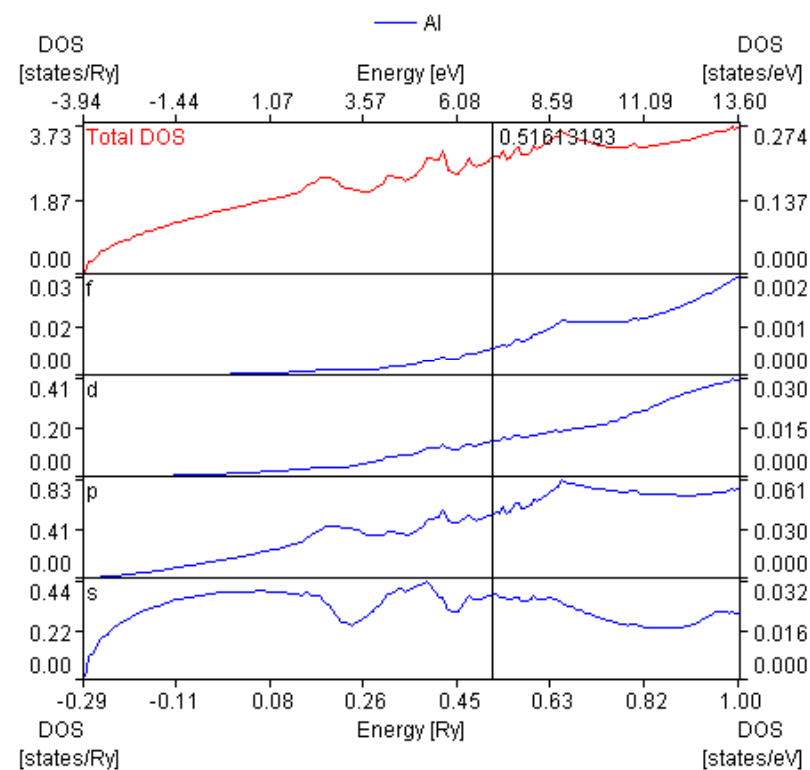
0.0155

Value max

40.8231

Density of States

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



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

The screenshot shows the CompoTherm software interface. On the left, the 'Dispersion Composites Design' window is active, displaying input fields for material ID, thermal conductivity, and dispersion parameters. A blue arrow points from this window to the right-hand window, which displays 'The calculated properties of composite'. This window shows the calculated thermal conductivity matrix at 300 K, diagonalization results, and principal axes vectors. A small 3D visualization of a composite structure is shown at the bottom of the right window.

Composite Design & Property Prediction System (CompoTherm)

The screenshot shows the Polymer Properties Prediction System software interface. On the left, the 'Modeling tool for Property Predictor' window is active, displaying a 3D molecular model of a polymer chain. A blue arrow points from this window to the right-hand window, which displays a table of predicted values for various properties. The table includes columns for Property, Unit, Value, and other parameters. A legend at the bottom of the table explains the symbols used in the predicted values.

Polymer Properties Prediction System

Composite Design & Property Prediction System (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.

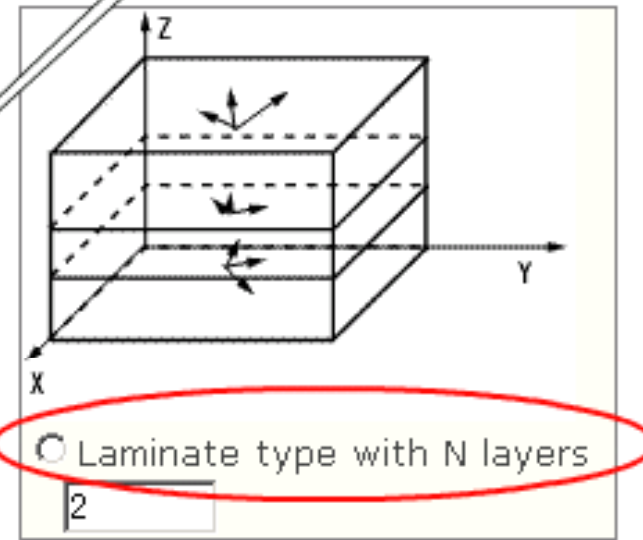
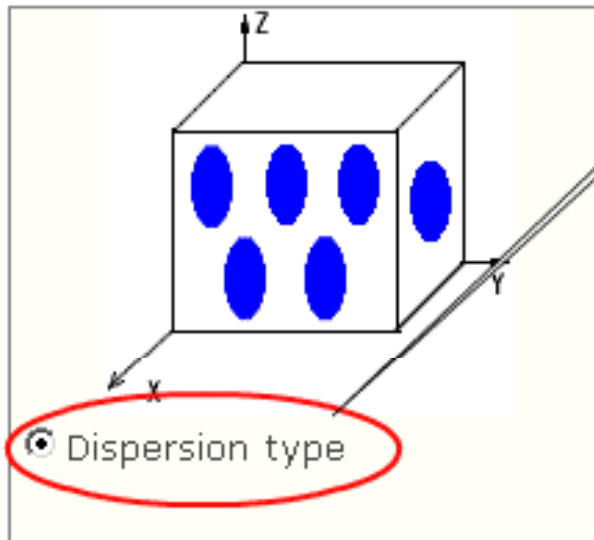
Calculate the density, specific heat, thermal conductivity and thermal diffusivity of the designed composites using the law of mixture, equivalent inclusion method and effective medium theory, etc. Easy modeling and quick calculation, suitable for investigating the dependence of thermo-physical properties on structure.

Thermo-physical property data of polymers, alloys and ceramics extracted from NIMS Materials Databases are available.



Structure type

Choose the structure type of composite material.



Select material type.

Reset >> Continue



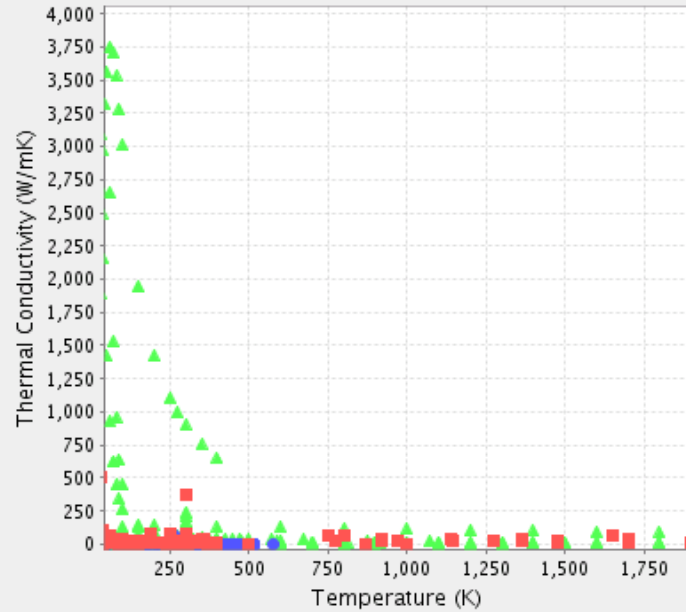
Copyright 2005 NIMS

Demonstration of the finite element analysis system screen on CompoTherm

Materials in Database

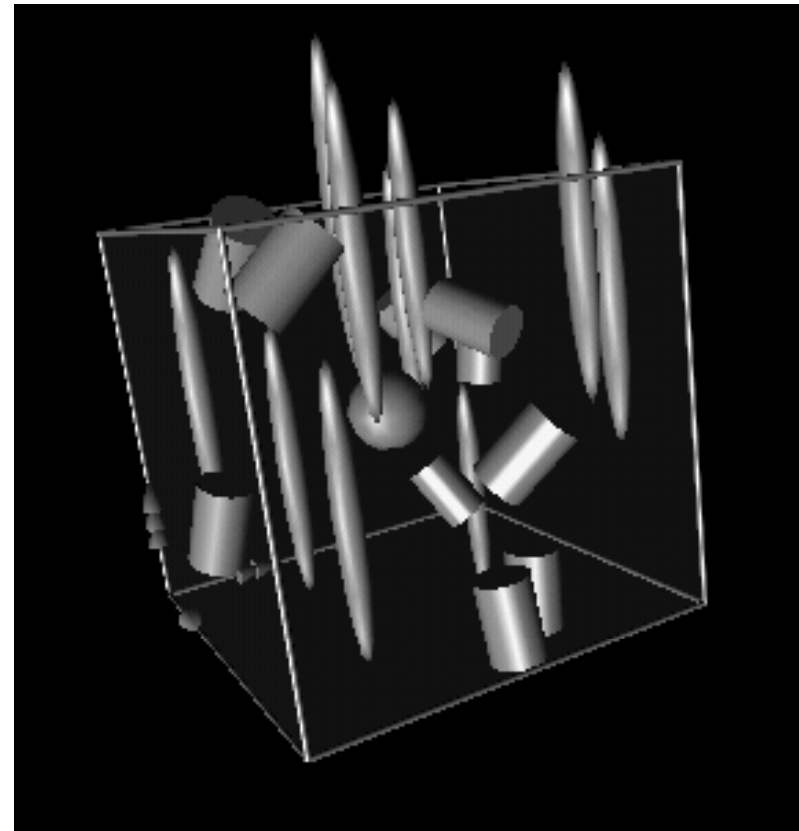
K vs T c vs T k vs c k vs p c vs p

Thermal conductivity vs Temperature



PaulingFile PolyInfo Other

temperature: (K)



3D model of a composite material case created by CompoTherm

Plot of the thermal conductivity of the thermal properties database

Metal Segregation Prediction System (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)

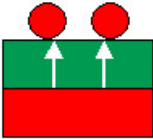
surface segregation in dilute alloy system (available in the future)

interface segregation at film-substrate interface (available in the future)

interface segregation at alloy-substrate interface (available in the future)

アドレス https://inaba.nims.go.jp/SurfSeg/select.html

移動 リンク 変換 選択



SurfSeg

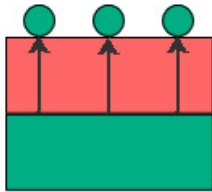
mits@ayamegusa.nims.go.jp NIMS MITS

[Home](#)
[Manual](#)

Segregation Simulation

choose a type of segregation

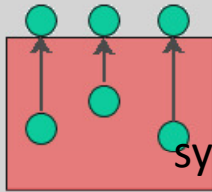
Under construction, will appear in future



Surface segregation
(film)

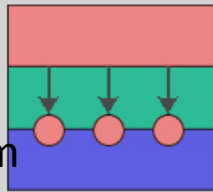
**in film/substrate
system**

Under construction, will appear in future



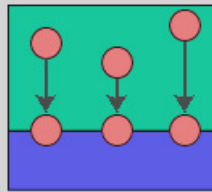
Surface segregation
(bulk)

in dilute
alloy system



Interface segregation
(film)

at film-substrate
interface system

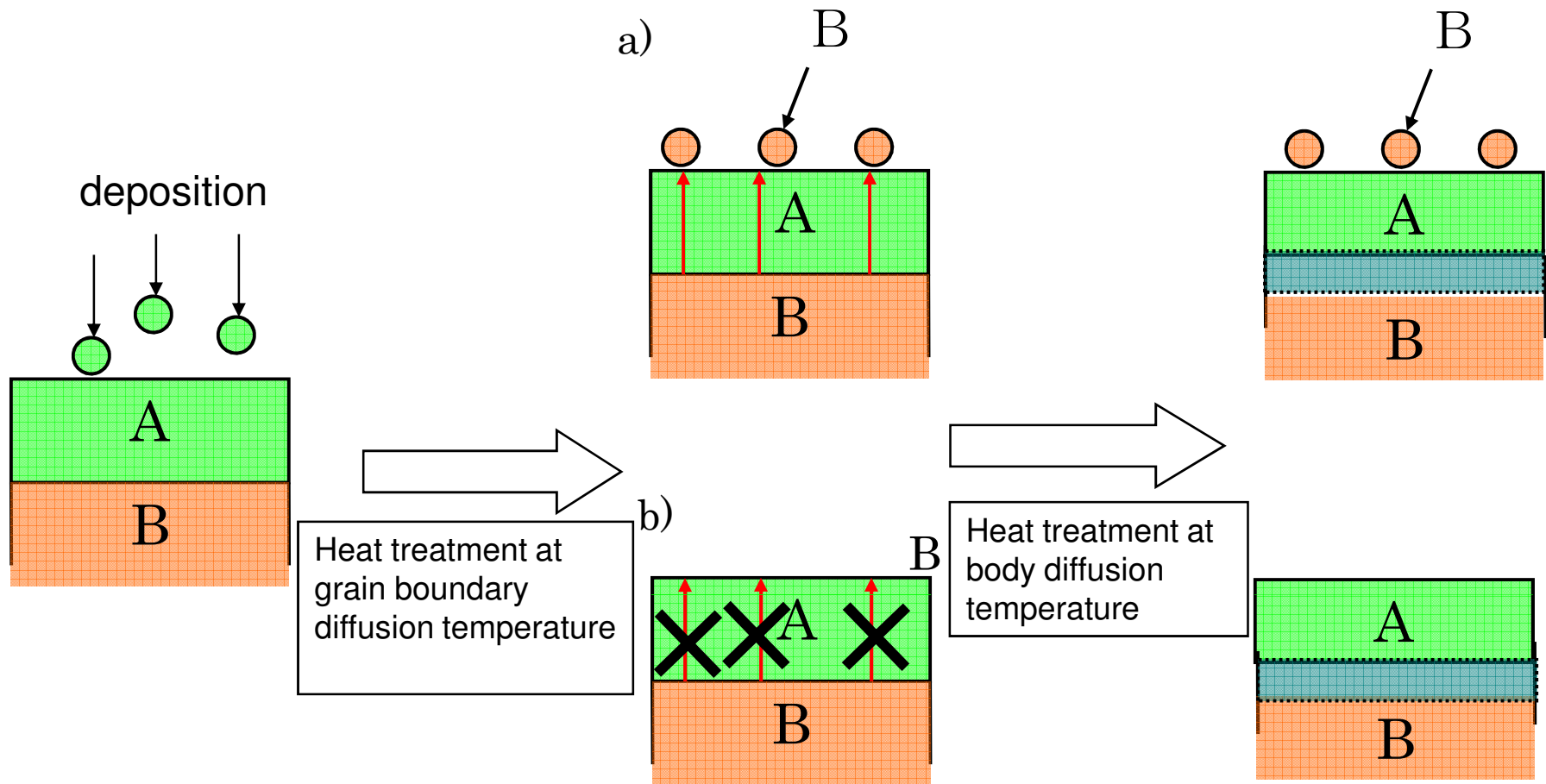


Interface segregation
(bulk)

at alloy-substrate
interface system

Copyright 2009 NIMS

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. finding a system which shows segregation of a desirable element.
2. Diffusion barrier: finding B that does not let A segregate on the surface. If A segregates on B, B is not suitable for diffusion barrier.

Select elements of each film and base from periodic table

First, select A or B, then choose element of A(substrate) or B (film) from the periodic table.

B (Film) Cu
 A (Substrate) Ti

Top

	1A	2A	3A	4A	5A	6A	7A	8	1B	2B	3B	4B	5B	6B	7B	0		
1	H																	
2	Li	Be								B	C	N	O	F	Ne			
3	Na	Mg								Al	Si	P	S	Cl	Ar			
4	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
6	Cs	Ba	L	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
7	Fr	Ra	A															
	L	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu		
	A	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr		

Available for combinations of 51 elements x 51 elements

Input screen

Click 'Calculate' and then results are shown

First, select A or B, then choose element of A(substrate) or B (film) from the periodic table.

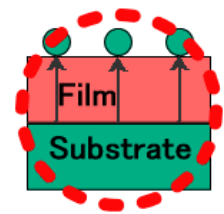
B (Film) Cu
 A (Substrate) Ti

Top

	1A	2A	3A	4A	5A	6A	7A	8	1B	2B	3B	4B	5B	6B	7B	0		
1	H																	
2	Li	Be								B	C	N	O	F	Ne			
3	Na	Mg								Al	Si	P	S	Cl	Ar			
4	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
6	Cs	Ba	L	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
7	Fr	Ra	A															
	L	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu		
	A	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr		

predicted results

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



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

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**The base of
COMPUTER NETWORK
is HUMAN NETWORK**



Thank you for your attention.

