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NIST Databases for Materials Research

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NIST Databases for Materials Research

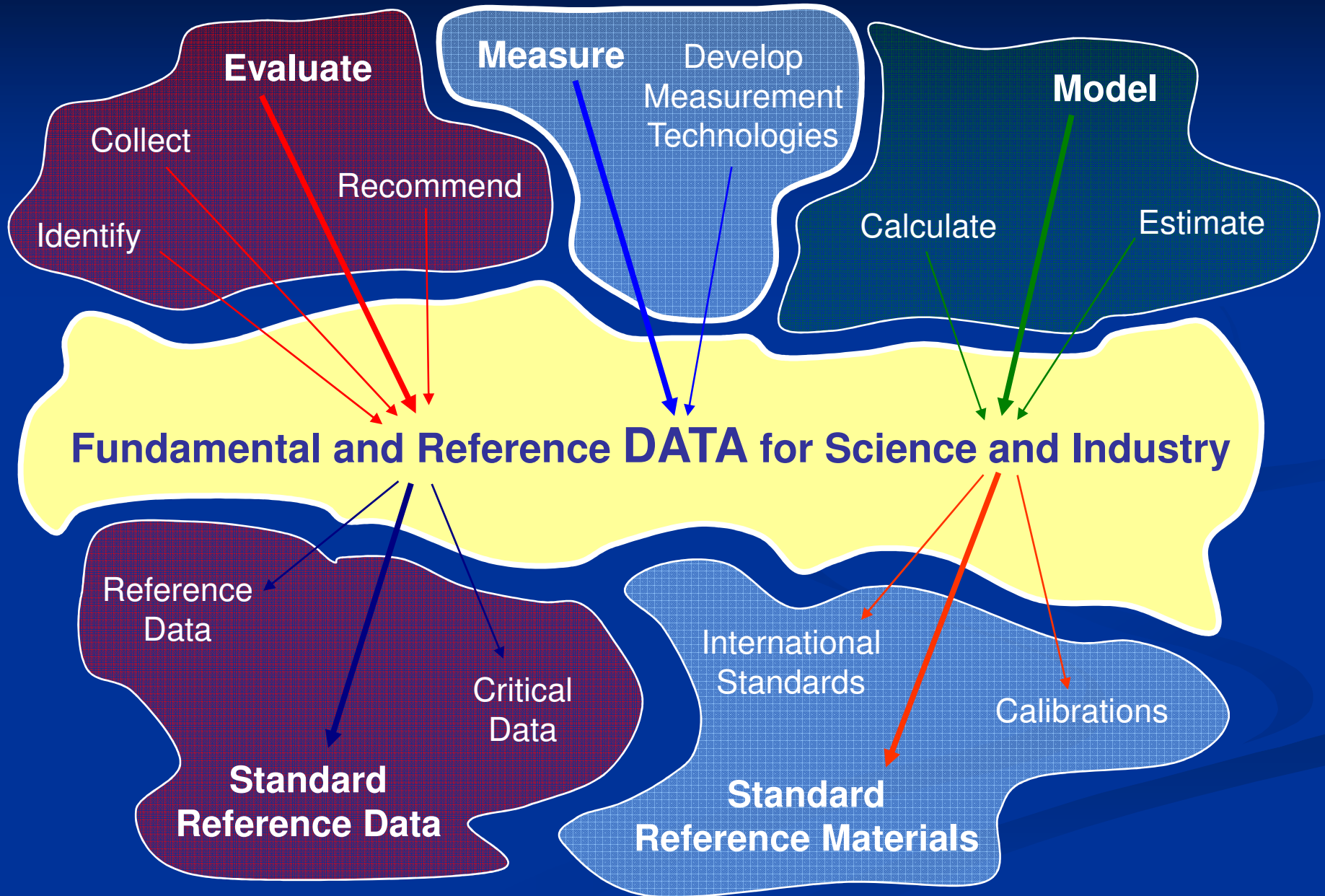
T. Vanderah, V. Karen, P. Linstrom, D. Burgess
(and others...)

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NIST Data Activities



NIST Role for Standards Setting Organizations

- NIST is a research agency that provides critical data and measurement technologies for use in science and industry
- NIST is not a standards setting body, but provides reference data for “realizing” standards which are formally adopted by standards setting organizations

- *The International Temperature Scale* (for example)
- ITS-90 is realized, maintained and disseminated by NIST to provide a standard scale of temperature and was adopted by the International Committee of Weights and Measures (*CIPM*) as the official international temperature scale on January 1, 1990
- NIST reference tables of thermocouple electromotive force (emf) versus temperature have been adopted as standards by the American Society for Testing and Materials (*ASTM*)

Standards Settings Bodies that Adopt NIST Realizations and Recommendations

- International Association for the Properties of Water and Steam (*IAPWS*)
- International Commission on Radiation Units & Measurements (*ICRU*)
- International Union for Pure and Applied Chemistry (*IUPAC*)
- Committee on Data for Science and Technology (*CODATA*)
- International Union for Pure and Applied Physics (*IUPAP*)
- General Conference on Weights and Measures (*CGPM*)
- International Bureau of Weights and Measures (*BIPM*)
- International Organization for Standardization (*ISO*)
- American Society for Testing and Materials (*ASTM*)
- American National Standards Institute (*ANSI*)
- International System of Units (*SI*)

NIST is a Primary Source of Reference Data

In addition to measuring, compiling, and evaluating critical reference data, NIST has published for over four decades much of the Standard Reference Data that is used in the physical and chemical sciences.

- *National Standard Reference Data Series (NSRDS): 1965-1987*
- *Journal of Physical and Chemical Reference Data (JPCRD): 1972-present*

Under the 1963 Standard Reference Data Act (Public Law 90-396) NIST has the primary responsibility in the Federal Government for providing reliable scientific and technical reference data.

CO

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Fundamental Physical Constants — Frequently used constants

Quantity	Symbol	Value	Unit	Relative std. uncert. u_r
speed of light in vacuum	c, c_0	299 792 458	m s^{-1}	(exact)
magnetic constant	μ_0	$4\pi \times 10^{-7}$ $= 12.566 370 614... \times 10^{-7}$	N A^{-2} N A^{-2}	(exact)
electric constant $1/\mu_0 c^2$	ϵ_0	$8.854 187 817... \times 10^{-12}$	F m^{-1}	(exact)
Newtonian constant of gravitation	G	$6.674 28(67) \times 10^{-11}$	$\text{m}^3 \text{kg}^{-1} \text{s}^{-2}$	1.0×10^{-4}
Planck constant	h	$6.626 068 96(33) \times 10^{-34}$	J s	5.0×10^{-8}
$h/2\pi$	\hbar	$1.054 571 628(53) \times 10^{-34}$	J s	5.0×10^{-8}
elementary charge	e	$1.602 176 487(40) \times 10^{-19}$	C	2.5×10^{-8}
magnetic flux quantum $h/2e$	Φ_0	$2.067 833 667(52) \times 10^{-15}$	Wb	2.5×10^{-8}
conductance quantum $2e^2/h$	G_0	$7.748 091 7004(53) \times 10^{-5}$	S	6.8×10^{-10}
electron mass	m_e	$9.109 382 15(45) \times 10^{-31}$	kg	5.0×10^{-8}
proton mass	m_p	$1.672 621 637(83) \times 10^{-27}$	kg	5.0×10^{-8}
proton-electron mass ratio	m_p/m_e	1836.152 672 47(80)		4.3×10^{-10}
fine-structure constant $e^2/4\pi\epsilon_0\hbar c$	α	$7.297 352 5376(50) \times 10^{-3}$		6.8×10^{-10}
inverse fine-structure constant	α^{-1}	137.035 999 679(94)		6.8×10^{-10}
Rydberg constant $\alpha^2 m_e c/2h$	R_∞	10 973 731.568 527(73)	m^{-1}	6.6×10^{-12}
Avogadro constant	N_A, L	$6.022 141 79(30) \times 10^{23}$	mol^{-1}	5.0×10^{-8}
Faraday constant $N_A e$	F	96 485.3399(24)	C mol^{-1}	2.5×10^{-8}
molar gas constant	R	8.314 472(15)	$\text{J mol}^{-1} \text{K}^{-1}$	1.7×10^{-6}
Boltzmann constant R/N_A	k	$1.380 6504(24) \times 10^{-23}$	J K^{-1}	1.7×10^{-6}
Stefan-Boltzmann constant $(\pi^2/60)k^4/\hbar^3 c^2$	σ	$5.670 400(40) \times 10^{-8}$	$\text{W m}^{-2} \text{K}^{-4}$	7.0×10^{-6}
Non-SI units accepted for use with the SI				
electron volt: $(e/C) \text{ J}$	eV	$1.602 176 487(40) \times 10^{-19}$	J	2.5×10^{-8}
(unified) atomic mass unit $1 \text{ u} = m_{\text{u}} = \frac{1}{12} m(^{12}\text{C})$ $= 10^{-3} \text{ kg mol}^{-1}/N_A$	u	$1.660 538 782(83) \times 10^{-27}$	kg	5.0×10^{-8}

NIST is
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NIST Data Products and Activities

- Online Databases
- Electronic Databases (PC)
- Print Databases

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- Calibrations

- Measurement Technologies

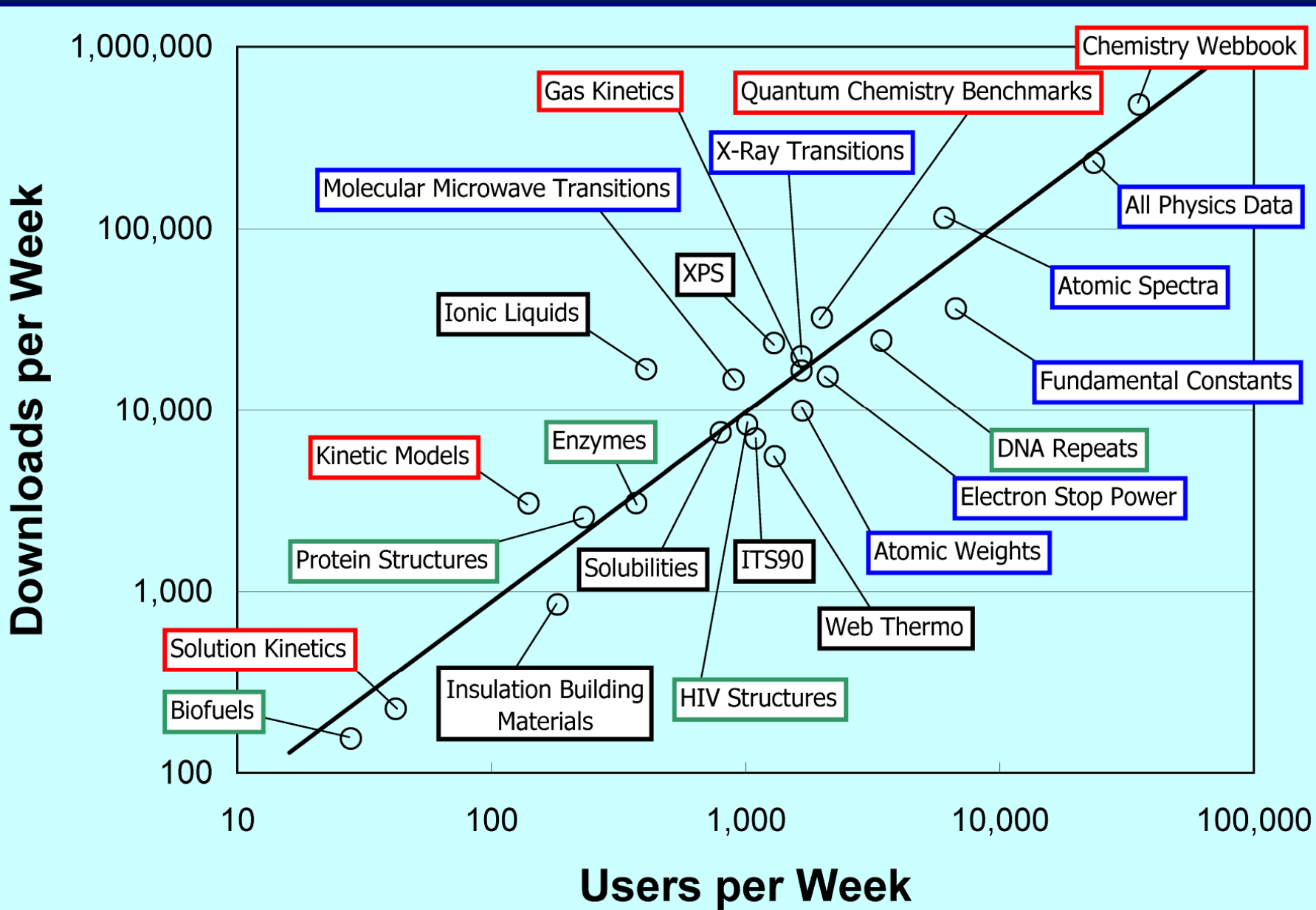
Some for *FREE*

Some for *FEE*

\$ nominal costs for distributing databases (~\$100-200)

\$\$\$ maintaining, expanding, and improving databases
(~\$1500-5000)

NIST Data Online



The NIST Data Gateway

<http://www.nist.gov/srd/>

The screenshot shows a web browser window with the address bar containing <http://www.nist.gov/srd/>. The browser's menu bar includes File, Edit, View, Favorites, Tools, and Help. The address bar also features a Live Search button. The browser's toolbar includes a home button, RSS feed icon, printer icon, page number, and a Tools menu. The website's header features the NIST logo, navigation links for NIST Time, NIST Home, About NIST, and Contact Us, and a search bar. Below the header is a navigation menu with links for Publications, Subject Areas, Products/Services, NIST Organization, News, Programs & Projects, and User Facilities. The main content area is titled "The NIST Data Gateway" and provides information about the gateway's purpose and search options. A sidebar on the left contains links to "About: Standard Reference Data (SRD)", "Standard Reference Data Act of 1968 (PL 90-396)", "Standard Reference Data Copyright Information", "NIST Online Databases List", "NIST Online Databases Descriptions", "Databases for Purchase", "Online Subscription Databases", "SRD Database Numbering System", and "NIST Databases Indexed by Discipline". A right sidebar includes a "Select Language" dropdown, a "Powered by Google Translate" notice, a "SHARE" button, and a "What's New in NIST Data" section with links to "Rate our Products and Services", "New Version, New Price, New Release", "Order SRD 31 NIST-ACerSPhase Equilibria Diagrams Database Now", "SRD 13 NIST-JANAF Thermochemical Tables", "SRD 1A NIST/EPA/NIH Mass Spectral Database NIST 11", "What's New in v.2.0g distributed with NIST 11", and "Click here for a list of our distributors." The footer of the right sidebar includes links for "NIST Standard Reference Database 203 Web Theme".

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The NIST Data Gateway

NIST Data Gateway-provides easy access to many (currently over 80) of the NIST scientific and technical databases. These databases cover a broad range of substances and properties from many different scientific disciplines. The Gateway includes links to free online NIST data systems as well as to information on NIST PC databases available for purchase.

To use the Gateway, select one of the following search options:

- Keyword
- Property
- Substance Name

Journal of Physical and Chemical Reference Data (JPCRD) is published by the American Institute of Physics (AIP) for NIST. The objective of the Journal is to provide critically evaluated physical and chemical property data, fully documented as to the original sources and the criteria used for evaluation.

- Journal of Physical and Chemical Reference Data
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SRD 1A NIST/EPA/NIH Mass Spectral Database NIST 11

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NIST Standard Reference Database 203 Web Theme



1. The DOE Office of Science and NSF will work together to enable the development, maintenance, and deployment of reliable, interoperable, and reusable software for the next-generation design of matter. The DOE, through its *Computational Materials and Chemistry by Design* program, and NSF, through aspects of its *Cyberinfrastructure Framework for 21st Century Science and Engineering*, will coordinate activities on the development of high quality production software toolkits that both incorporate new algorithms and allow for interoperability with existing software tools.
2. In support of their advanced software programs, both the DOE and NSF will also coordinate activity in the development of next-generation characterization tools that provide the fundamental basis for development of and validation of the algorithms and software tools.
3. An *Advanced Materials by Design* program led by NIST will target the development of standards infrastructure, reference databases, and centers of excellence that will enable reliable computer modeling and simulation for materials discovery and optimization. This activity will be coordinated closely with the DOE and NSF efforts on software and experimental tool design.

Achieving the Vision

Next Steps

5. NSF and DOD will play a lead role in addressing the next-generation workforce goals by: facilitating new partnerships between the relevant science and engineering communities in academia, government and industry to promote a culture supporting and embracing the use of the capabilities developed within this initiative; and engaging with students and colleagues to develop the culture and relevant training of the next-generation workforce.
6. NSF and DOD will play a lead role in addressing the next-generation workforce goals by: facilitating new partnerships between the relevant science and engineering communities in academia, government and industry to promote a culture supporting and embracing the use of the capabilities developed within this initiative; and engaging with students and colleagues to develop the culture and relevant training of the next-generation workforce.



© Robert Rathe

Phase Equilibria Diagrams Database

NIST SRD 31: <http://www.nist.gov/srd/nist31.cfm>

- Began in 1933 via NIST-ACerS collaboration

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

By F. P. HALL and HERBERT INSLEY

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

Use of Phase Equilibria Diagrams

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

Phase Equilibria Diagrams Database

NIST SRD 31: <http://www.nist.gov/srd/nist31.cfm>

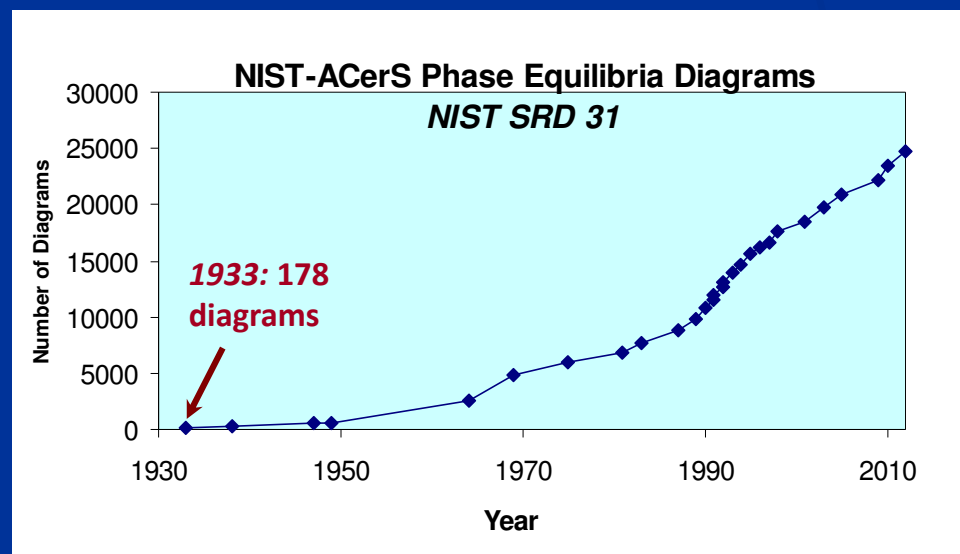
- Numerous material-system classes
 - oxides
 - salts, halides
 - borides, carbides, silicides
 - pnictides: nitrides, phosphides, arsenides
 - chalcogenides, semiconductors: sulfides, selenides, tellurides

- Continuous growth:
~ 1,000 diagrams per year

- Published data:
 - 18,000 figures with
~ 26,000 diagrams

- Unpublished data:
 - ~ 25,000 entries with
~ 50,000 diagrams

- sorted/searchable by chemical system
- "INFO" file of ~ 6,000 literature references



contact: terrell.vanderah@nist.gov

Phase Equilibria Diagrams Database

NIST SRD 31: <http://www.nist.gov/srd/nist31.cfm>

Data Center Process

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

http://www.nist.gov/srd/nist31.cfm

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http://www.nist.gov/srd/nist31.cfm

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- Biotechnology
- Chemical and Crystal Structure
- Chemical Kinetics
- Chemistry
- Communications
- Construction
- Environmental Data
- Fire
- Fluids
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- Materials Properties
- Mathematical Databases, Software and Tools
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New release, Version 3.4

NIST Standard Reference Database 31

ACerS-NIST Phase Equilibria Diagrams Database:
(formerly known as *Phase Diagrams for Ceramists*)

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7:37 PM

Phase Equilibria Diagrams Database

NIST SRD 31: <http://www.nist.gov/srd/nist31.cfm>

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

Phase Diagrams CD ROM Application


File Search List Window Help

Commentaries and Diagrams Search

Search By Components or Elements

Equals Containing all (and only) Containing any (but nothing else) Containing

BaO-TiO2

Chemical Component List: --Choose a Component-- Periodic Table: 

Not Containing:

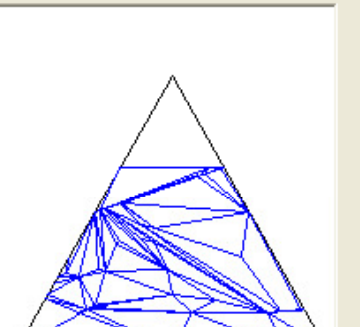
Volume No: All Volumes Language: All

Publication Year: Between And Author's Last Name:

Figure No. Equals: Include Info. Ref.

Phase Vol.	Fig. No.	Chemical System	Authors	Pub Year
<input type="checkbox"/> Annual-93	93-238	BaO-Ti2O3-NbO2-TiO2-Nb2O5	G. V. Bois, V. I. Zhuk...	1976
<input type="checkbox"/> Annual-93	93-016	BaO-TiO2	H. M. O'Bryan, J. Th...	1983
<input type="checkbox"/> 08	07975	BaO-SiO2-TiO2-H2O	B. Yu. Komilovich, N...	1981
<input type="checkbox"/> 12	10036	BaO-Fe2O3-TiO2	T. A. Vanderah, J. M...	1996
<input type="checkbox"/> 03	04302	BaO-TiO2	T. Negas, R. S. Roth...	1974
<input type="checkbox"/> 03	04545	BaO-B2O3-TiO2	Y. Goto, L. E. Cross	1969
<input type="checkbox"/> 04	05135	BaO-TiO2	H. M. O'Bryan, Jr., J. ...	1974
<input type="checkbox"/> 04	05369	BaO-CeO2-TiO2	J. P. Guha, D. Kolar	1973
<input type="checkbox"/> 04	05371	BaO-GeO2-TiO2	J. P. Guha, D. Kolar	1972
<input type="checkbox"/> 04	05455	Na2O-BaO-TiO2-Nb2O5	Y. Itoh, H. Iwasaki	1972

Record(s): 135



Periodic Table

Chemical components (elements) to be searched:

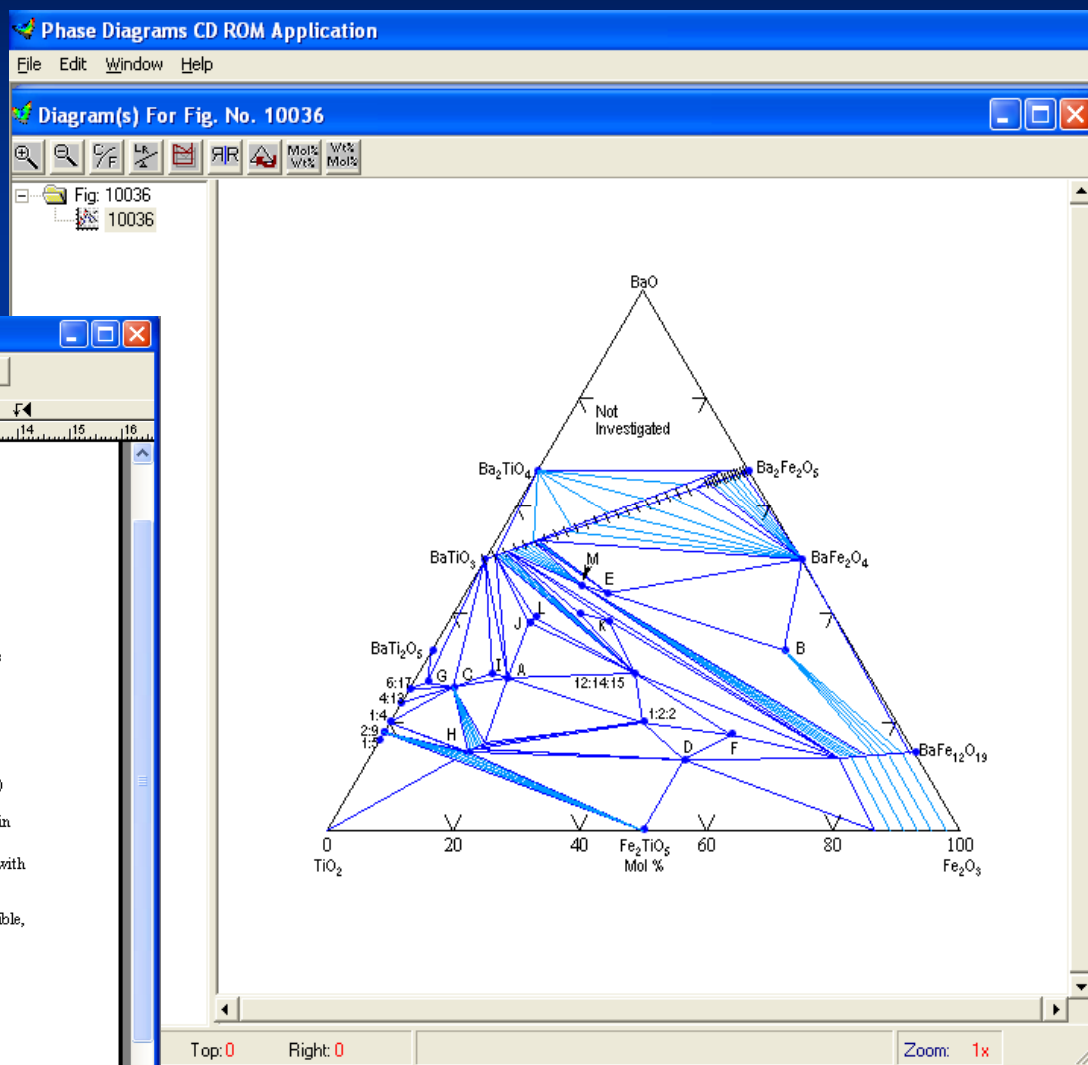
BaO-TiO2

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

Phase Equilibria Diagrams Database

NIST SRD 31: <http://www.nist.gov/srd/nist31.cfm>

■ Display: Phase Diagram and Commentary data



Commentary For Fig. No. 10036

BaO-Fe₂O₃-TiO₂

Fig. 10036—System TiO₂-BaO-Fe₂O₃. Solid state compatibility at 1250°-1270°C in air. A = Ba₂Fe₂Ti₄O₁₃; B = Ba₃Fe₁₀TiO₂₀; C = Ba₄Fe₂Ti₁₀O₂₇; D = Ba₃Fe₂₄Ti₇O₅₃; E = Ba₄Fe₄Ti₃O₁₆; F = Ba₂Fe₁₂Ti₃O₂₆; G = Ba₁₄Fe₂Ti₃₅O₈₇; H = hollandite, Ba_xFe_{2x}Ti_{8-2x}O₁₆ (1.35 ≤ x ≤ 1.55); I = Ba₃Fe₆Ti₁₆O₄₉; J = Ba₃Fe₂Ti₄O₁₄; K = Ba₃Fe₁₀Ti₈O₃₉; L = Ba₆Fe₄Ti₇O₂₆; M = Ba₃Fe₆Ti₆O₂₉; N = Ba₂Fe₂Ti₂O₉; 1:2:2 = BaFe₄Ti₂O₁₁; 12:14:15 = Ba₁₂Fe₂₈Ti₁₅O₈₄.

T. A. Vanderah, J. M. Loezos, and R. S. Roth, *J. Solid State Chem.*, **121** [1] 38-50 (1996).

Approximately 150 compositions were studied in this system. Starting materials were AR BaCO₃, AR Fe₂O₃, and "phosphate-free" TiO₂. Samples were ground in an agate mortar for 15-20 min before being pressed into pellets. Pellets, placed on powders of the same composition, were heat treated at 1000°C (48 h) prior to multiple heatings at 1250°-1270°C, each 1 week duration, all in air. Samples were step-cooled to 750°C and air quenched to room temperature. Equilibrium was attained when no further change was noted in the X-ray diffraction results, typically 3-5 heatings.

Only the 1:2:2,^{1,2} 12:14:15,³ and hollandites were previously reported. In the present work, all phases (with the exception of "N") were characterized for crystal type and unit cell parameters. These are collected in the present work. Single-crystal growth experiments were attempted using both neat melts and also using K₂O-B₂O₃ fluxes. The former experiments were most successful on melts cooled at 1°C/h. Wherever possible, X-ray powder diffraction data were indexed using lattice parameters derived from precession X-ray photographs of melt-grown single crystals.

1. F. Habery and M. Velicescu, *Acta Crystallogr., Sect. B: Struct. Crystallogr. Cryst. Chem.*, **B30** [Pt. 6] 1507-1510 (1974).
2. X. Obradors, A. Collomb, J. Pannetier, A. Isalgue, J. Tejada, and J. C. Joubert, *Mater. Res. Bull.*, **18** [12] 1543-1553 (1983).
3. I. E. Grey, A. Collomb, and X. Obradors, *J. Solid State Chem.*, **91** [1] 131-139 (1991).

A.E.M.

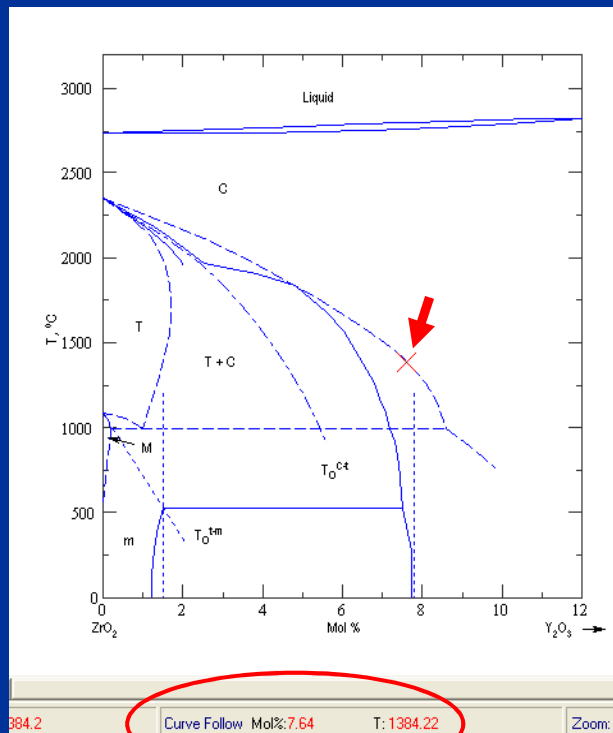
Page 1 Line 1 Col 0 100 % NUM

Phase Equilibria Diagrams Database

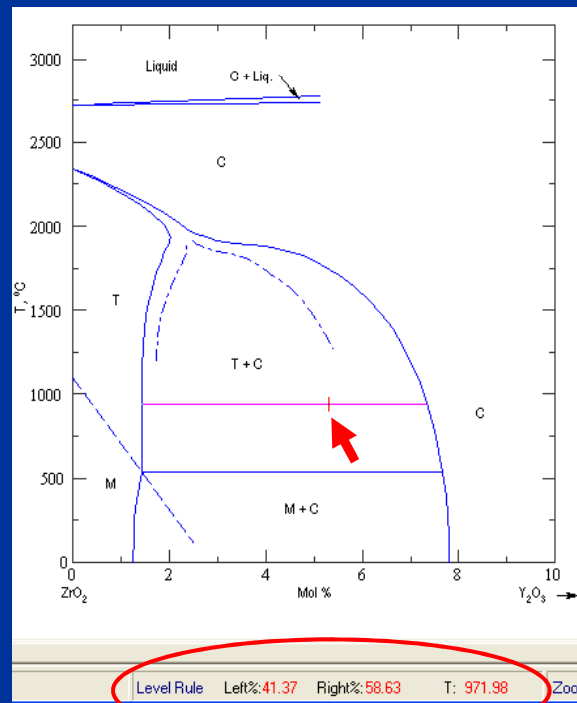
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- Built-in functions allow user to track coordinates, zoom, convert mol% \leftrightarrow wt%, use level rule, overlay diagrams, rotate ternaries

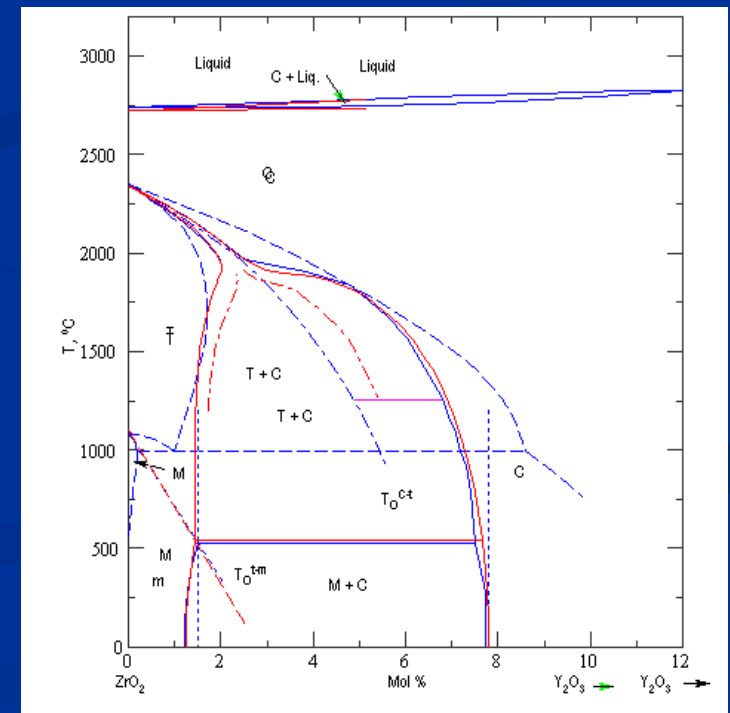
Curve Follow



Lever Rule



Overlay Diagrams



- Price recently reduced by ~2/3 (\$3K → \$950)
- Recent investments: >\$0.5 M, all-new software, hardware, physical space

NIST Standard Reference Database 31

ACerS-NIST Phase Equilibria Diagrams Database

New Release, Version 3.4

**New release
New, lower price**



892 new entries

1,400 new diagrams

24,800 total diagrams

<http://www.nist.gov/srd/nist31.cfm>

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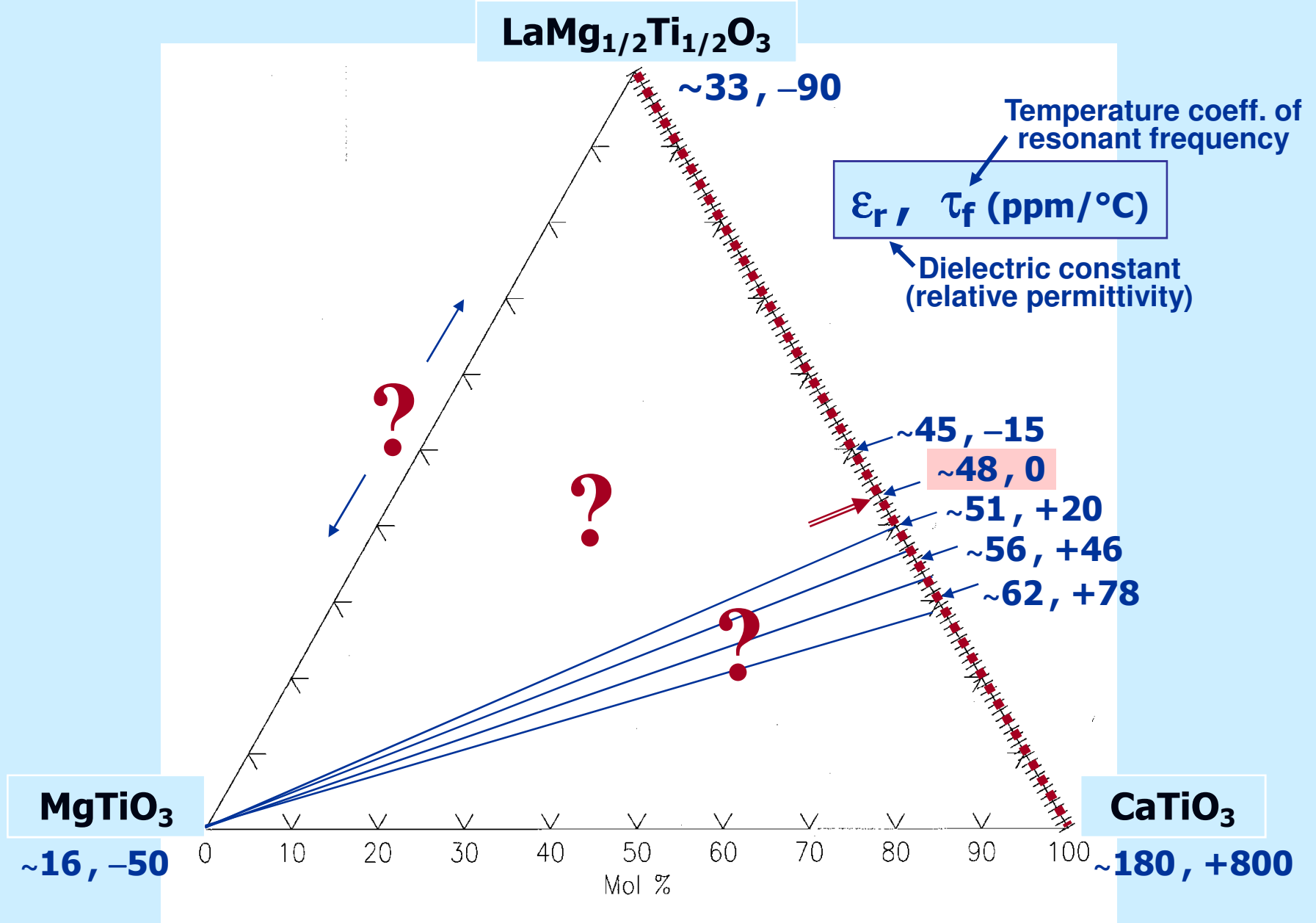
Rational Processing

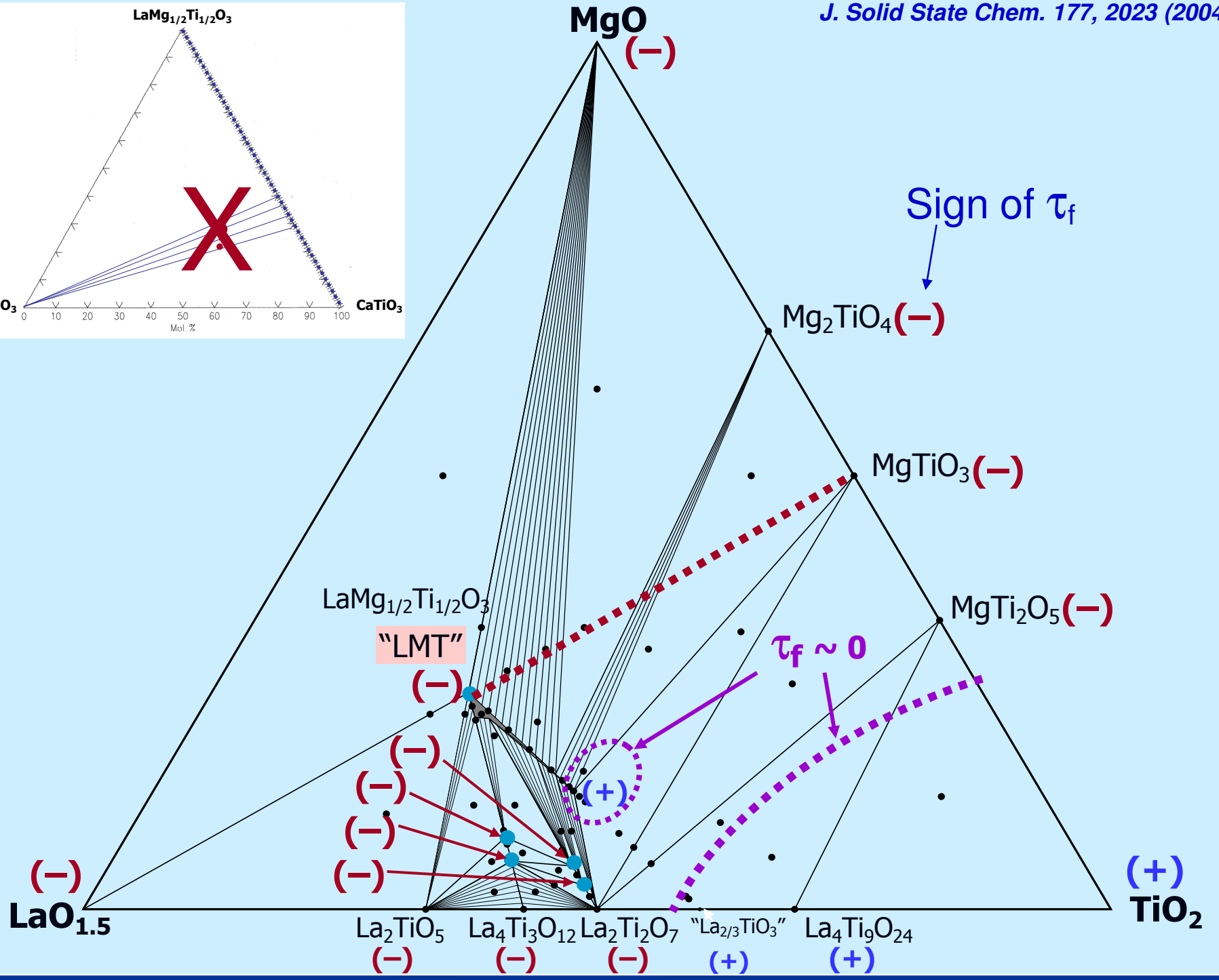
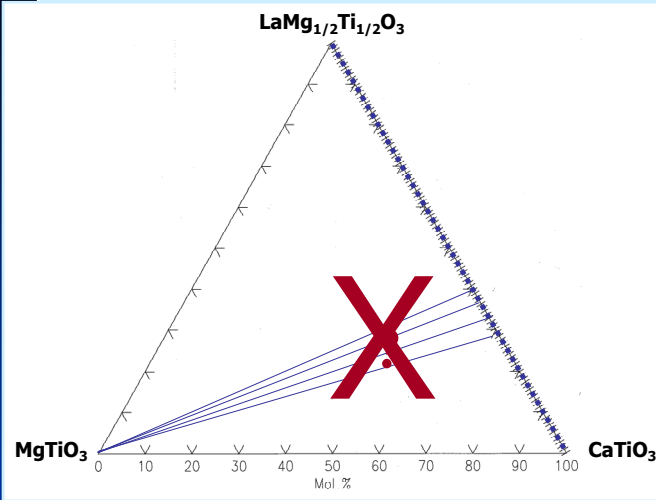
- Reliable phase equilibrium diagrams are particularly useful when the exploitable properties are **additive**.
- Example: microwave dielectric ceramics

$44\text{LaMg}_{1/2}\text{Ti}_{1/2}\text{O}_3 - 56\text{CaTiO}_3$ solid solution

- *of interest for resonators/filters*
- *dielectric constant ~ 48 , temperature coefficient_(f) ~ 0*
- **\rightarrow need to improve dielectric loss**

LaMg_{1/2}Ti_{1/2}O₃-CaTiO₃ solid solution





NIST Crystallographic Databases

- NIST Standard Reference Databases:
 - SRD 3: NIST Crystal Data (~237,000 entries)
 - Inorganic and organic crystalline materials
 - Crystallographic information without atomic coordinates
 - SRD 83: NIST Structural Database (~60,000 entries)
 - Metals and inter-metallics
 - Atomic coordinates and structure types
 - SRD 84: FIZ/NIST Inorganic Crystal Structure Database (ICSD, ~150,000 entries)
 - Inorganic materials
 - Refined structure information

contact: vicky.karen@nist.gov

FIZ-NIST Inorganic Crystal Structure Database

ICSD 150,042 entries, Release 2012-1

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



<http://www.nist.gov/srd/nist84.cfm>

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Symmetry
Reference

↓ ↓		<table border="1" style="width: 100%; border-collapse: collapse;"> <tr> <td style="background-color: #e0f0ff;">MET</td> <td style="background-color: #e0f0ff;">TRM</td> <td style="background-color: #e0f0ff;">NOM</td> <td colspan="7"></td> </tr> <tr> <td style="background-color: #e0f0ff;">TRU</td> <td style="background-color: #e0f0ff;">ALE</td> <td style="background-color: #e0f0ff;">CHA</td> <td colspan="7"></td> </tr> </table>										MET	TRM	NOM								TRU	ALE	CHA								↓										
MET	TRM	NOM																																								
TRU	ALE	CHA																																								
H	D	T											He																													
Li	Be											Ne																														
Na	Mg											Ar																														
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr																									
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe																									
Cs	Ba	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn																										
Fr	Ra	Rf	Ha																																							
		<table border="1" style="width: 100%; border-collapse: collapse;"> <tr> <td style="background-color: #ffe0e0;">La</td><td style="background-color: #ffe0e0;">Ce</td><td style="background-color: #ffe0e0;">Pr</td><td style="background-color: #ffe0e0;">Nd</td><td style="background-color: #ffe0e0;">Pm</td><td style="background-color: #ffe0e0;">Sm</td><td style="background-color: #ffe0e0;">Eu</td><td style="background-color: #ffe0e0;">Gd</td><td style="background-color: #ffe0e0;">Tb</td><td style="background-color: #ffe0e0;">Dy</td><td style="background-color: #ffe0e0;">Ho</td><td style="background-color: #ffe0e0;">Er</td><td style="background-color: #ffe0e0;">Tm</td><td style="background-color: #ffe0e0;">Yb</td><td style="background-color: #ffe0e0;">Lu</td> </tr> <tr> <td style="background-color: #ffe0e0;">Ac</td><td style="background-color: #ffe0e0;">Th</td><td style="background-color: #ffe0e0;">Pa</td><td style="background-color: #ffe0e0;">U</td><td style="background-color: #ffe0e0;">Np</td><td style="background-color: #ffe0e0;">Pu</td><td style="background-color: #ffe0e0;">Am</td><td style="background-color: #ffe0e0;">Cm</td><td style="background-color: #ffe0e0;">Bk</td><td style="background-color: #ffe0e0;">Cf</td><td style="background-color: #ffe0e0;">Es</td><td style="background-color: #ffe0e0;">Fm</td><td style="background-color: #ffe0e0;">Md</td><td style="background-color: #ffe0e0;">No</td><td style="background-color: #ffe0e0;">Lr</td> </tr> </table>										La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr	
La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu																												
Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr																												

And And Not
 Or Or Not

AND Element Count: to
 Element Subscri: to
 Oxidation State: to

Type

 Normal
 Exclusive AND
 Exclusive OR

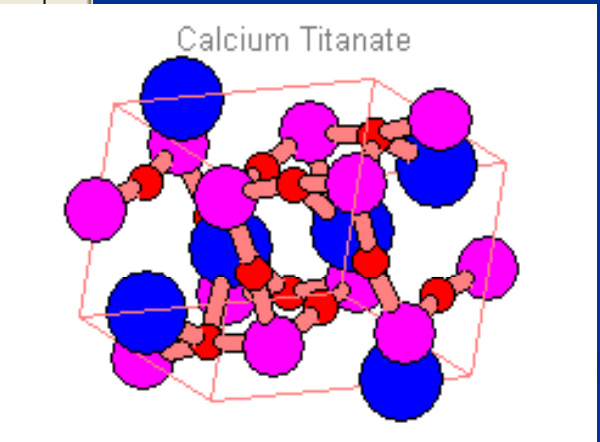
Selected Elements: (Boolean operators are in the upper right. Right click on groups to see contents.)

(0 AND Ca AND Ti)

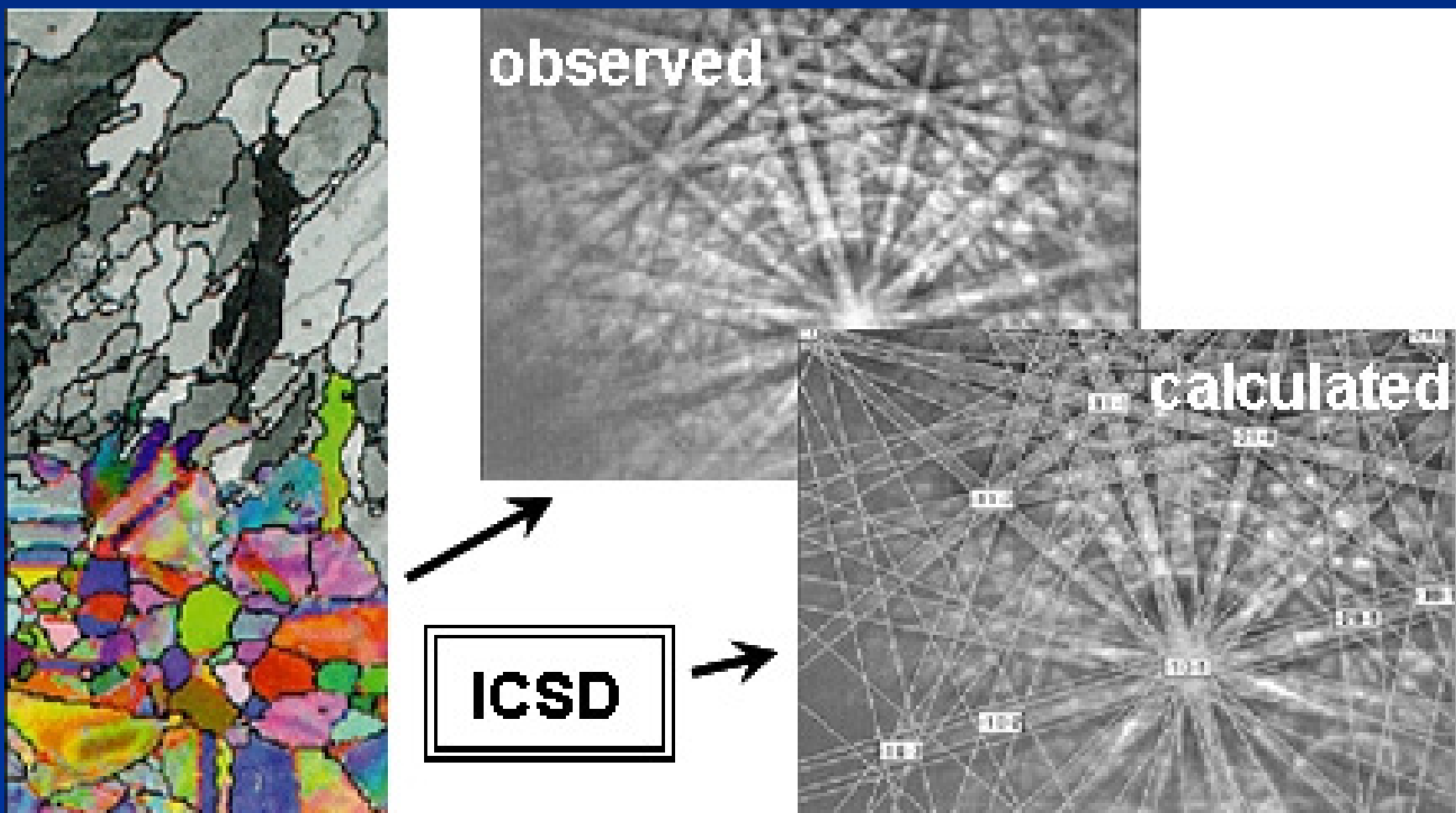
Calcium Titanate [Power Simulation]
✕

Home
Back
Forward
Stop
Zoom In
Zoom Out
XY
Print

2θ



SRD 84 ICSD: Phase Identification by Electron Diffraction



SRD 84 ICSD: Phase Identification by Electron Diffraction

HKL Flamenco - Setup

Project Edit View Calibration EBSP Job Tools Windows Help

Imaging Setup Interactive Automatic

75%

Snap EBSP Detect bands Index

Tilt: 70°
kV: 20
Mag: 500x

Simulation

Frozen SEM Image Live EBSP EBSP Geometry Band Detection Solution Simulation Image Storage

Properties

Match Unit: Si

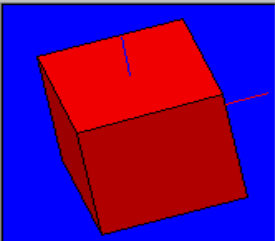
Method: Euler Angles

Euler Angles:
 ϕ_1 : 191.723
 Φ : 51.838
 ϕ_2 : 188.105

Current solution

Background:
 Current EBSP
 Color: Blue
 Show previous

Unit cell [Acq. surface]:



dG = 0.00°

R:n/a G:n/a B:n/a

Phases

Add... Remove

Max. number of reflectors: 50

Phases for indexing: 8 active (of PS F5)

<input checked="" type="checkbox"/>	Si	+ ϕ
<input checked="" type="checkbox"/>	Si	+ ϕ
<input checked="" type="checkbox"/>	Si	+ ϕ
<input checked="" type="checkbox"/>	Si	+ ϕ
<input checked="" type="checkbox"/>	Si	+ ϕ
<input checked="" type="checkbox"/>	Si	+ ϕ
<input checked="" type="checkbox"/>	Si	+ ϕ
<input checked="" type="checkbox"/>	Si	+ ϕ

[Phase information]
 Name=Si
 Source=Science [SCIEAS], (1963).
 Database=NIST Structural Database
 SpaceGroup=141
 LaueGroup=5, 4/mmm
 UnitCellLengths=4.69, 4.69, 2.59 Å
 UnitCellAngles=90.0, 90.0, 90.0 °
 Composition=Si(100 at%)

[Reflectors]
 Count= 50

#	(h k l)	Intensity
1.	(2 0 0)	100.0%
2.	(0 2 0)	100.0%
3.	(0 1 1)	45.9%
4.	(1 0 1)	45.9%
5.	(1 0 -1)	45.9%
6.	(0 1 -1)	45.9%
7.	(2 2 0)	40.0%
8.	(-2 -2 0)	40.0%
9.	(1 -2 -1)	19.1%
10.	(1 -2 1)	19.1%
11.	(1 2 1)	19.1%

NIST structural database, HKL Phases

Settings... Search

Elements: Si

Search result: 9 phases found. 0.03 s

Si(Si 100%)
 Si(Si 100%)
 Si(Si 100%)
 Si(Si 100%)
 Si(Si 100%)
 Ce O_s2 Si2 (Si 100%)
 Si(Si 100%)

[Phase information]
 Name=Si
 Source=Jpn. J. Appl. Phys. Part 1 [J.
 Database=NIST structural database
 SpaceGroup=227, F d -3 m
 LaueGroup=11, m3m
 UnitCellLengths=5.43, 5.43, 5.43 Å
 UnitCellAngles=90.0, 90.0, 90.0 °
 UnitCellVolume=160.10 Å³
 PhaseFamily=14 - best in family

[Elements, atom%]
 Summary=Si 100%
 Silicon 100%

[Reflectors]
 # (h k l) Intensity

#	(h k l)	Intensity
1.	(1 -1 -1)	100.0%
2.	(1 1 -1)	100.0%
3.	(1 1 1)	100.0%
4.	(1 -1 1)	100.0%
5.	(2 -2 0)	65.5%
6.	(2 0 -2)	65.5%
7.	(0 2 -2)	65.5%

Vision of Crystallographic Database Applications in MGI

- **What can we do with the Crystallographic Databases:**
 - **Provide initial guidance in the designing stage**
 - Select materials based on known chemical/structural/symmetrical criteria.
 - *ab initio* calculation of properties using database information.
 - Data-mining and other methods for locating potential candidates.
 - **High-throughput phase identification in the experimental stage**
 - Lattice matching
 - Powder diffraction fingerprinting
 - Lattice-fringe fingerprinting
 - **Input for scientific simulation**, interfacing with other computational tools for data analysis and knowledge discovery.

New effort (2013): NIST Crystallographic Database Design to Accommodate MGI: *Intelligent Access to SRD 84*

More User Definable Views
....

Chemistry View

Literature View

Symmetry View

Application View

Relate Tables

Chemistry Reference Density Atomic Positions Cell Parameters
Literature Data

Reduced cell
Derived Data

MATERIALS PROJECT

A Materials Genome
Approach

*Accelerating materials discovery through
advanced scientific computing and
innovative design tools.*

Search powered by **MOOGLE**

Database Statistics

26140 materials **3044** bandstructures
389 intercalation batteries **13381** conversion batteries

Register now for free, full access.

- Unlimited access
- Up to 500 search results
- History of your searches and analyses

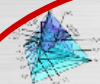
Or try the apps in demo mode

- 10 minute usage limit
- Search results limited to 10 best matches
- Just click an app to start



Materials Explorer

Search for materials information by chemistry, composition, or property.



Phase Diagram App

Computational phase diagrams for closed and open systems. Find stable phases and study



Lithium Battery Explorer

Find candidate materials for lithium batteries. Get voltage profiles and oxygen evolution data.



Reaction Calculator

Calculate the enthalpy of tens of thousands of reactions and compare with experimental



Crystal Toolkit

Convert between CIF and VASP input files. Generate new crystals by substituting or removing species.



Structure Predictor

Predict new compounds using data-mined substitution algorithms.



Page Discussion

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Phase Diagram App Manual

Contents [hide]

- 1 Introduction
- 2 Using the Computational Phase Diagram App
- 3 Interpreting Phase Diagrams
 - 3.1 Basic Phase Diagram Information
 - 3.2 Compositional Phase Diagrams
 - 3.2.1 Binary Compositional Phase Diagrams
 - 3.2.2 Ternary Compositional Phase Diagrams
 - 3.2.3 Quaternary Compositional Phase Diagrams
 - 3.3 Grand Potential Phase Diagrams
- 4 Accuracy of Calculated Phase Diagrams
- 5 Thermodynamics Methodology
 - 5.1 Compositional Phase Diagrams
 - 5.2 Grand Potential Phase Diagrams
- 6 Other Resources
- 7 Citation
- 8 References
- 9 Authors

Introduction

Phase diagrams represent the thermodynamic aspects regarding the processing of a material during a consuming process, requiring careful interpretation. Computational tools can accelerate

Using the above assumption, the effect of temperature and partial pressure can be fully captured in a single chemical potential variable, with a more negative value corresponding to higher temperatures or lower partial pressures. The chemical potential is then treated as an external variable to obtain a grand potential phase diagram under a particular condition by taking the convex hull of $\bar{\phi}$ for all phases and projecting the stable nodes into the Li-Fe composition space.

Other Resources

1. [Matlab package](#) developed by this author (S.P. Ong) to generate publication-quality figures from a csv data file.

Citation

To cite the Computational Phase Diagram App, please reference the following works:

- S. P. Ong, L. Wang, B. Kang, G. Ceder., The Li-Fe-P-O₂ Phase Diagram from First Principles Calculations, Chemistry of Materials, vol. 20, Mar. 2008, pp. 1798-1807.
- S.P. Ong, A. Jain, G. Hautier, B. Kang, and G. Ceder, Thermal stabilities of delithiated olivine MPO₄ (M=Fe, Mn) cathodes investigated using first principles calculations, Electrochemistry Communications, vol. 12, 2010, pp. 427-430.

References

1. [↑](#) NIST Chemistry WebBook, NIST Standard Reference Database Number 69, Eds. P.J. Linstrom and W.G. Mallard.
2. [↑](#) [2.0.2.1.2.2](#) S. P. Ong, L. Wang, B. Kang, G. Ceder., The Li-Fe-P-O₂ Phase Diagram from First Principles Calculations, Chemistry of Materials, vol. 20, Mar. 2008, pp. 1798-1807.
3. [↑](#) [3.0.3.1.3.2](#) S.P. Ong, A. Jain, G. Hautier, B. Kang, and G. Ceder, Thermal stabilities of delithiated olivine MPO₄ (M=Fe, Mn) cathodes investigated using first principles calculations, Electrochemistry Communications, vol. 12, 2010, pp. 427-430.
4. [↑](#) V. Raghavan, Fe-Li-O Phase Diagram, ASM Alloy Phase Diagrams Center, P. Villars, editor-in-chief, H. Okamoto and K. Cenzual, section editors; <http://www1.asminternational.org/AsmEnterprise/APD>, ASM International, Materials Park, OH, 2006.
5. [↑](#) C. B. Barber, D. P. Dobkin, & H. Huhdanpaa, 1996. The quickhull algorithm for convex hulls. ACM Transactions on Mathematical Software (TOMS), 22(4), p.469.

Authors

1. Shyue Ping Ong
2. Anubhav Jain

Navigation

Wiki home
Recent changes
Random page
Help
Materials Project portal

Toolbox

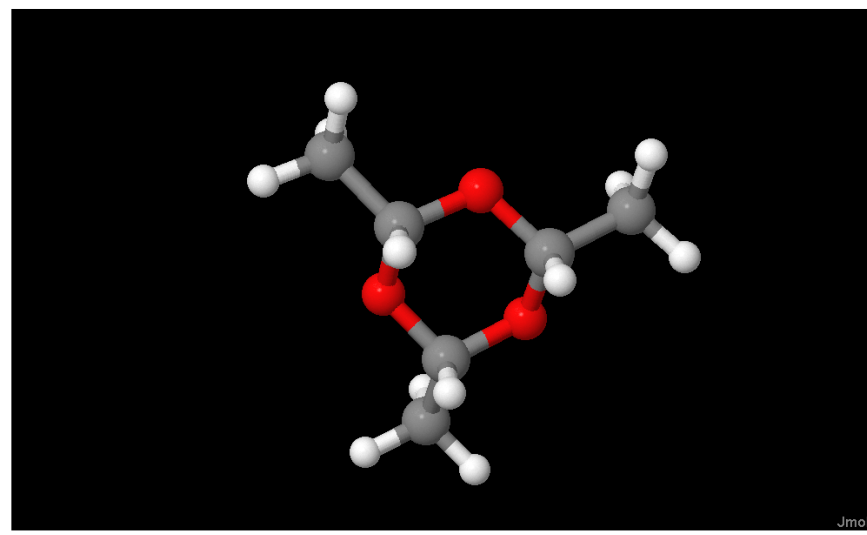
What links here
Related changes
Special pages
Printable version
Permanent link

The NIST Chemistry WebBook (SRD 69)

- Most widely used NIST data product
- Contains an extensive set of data for over 70,000 molecular species – *online since 1997 (!)*
 - Thermochemical and thermophysical properties
 - IR, UV/Vis, electronic and mass spectra
 - Ion and ion-cluster data
- Collects data from many NIST and non-NIST sources in one spot
- Used 24/7 worldwide - ~6,500 people a day
- 3-D structures can now be viewed online
- peter.linstrom@nist.gov



Structure for Paraldehyde



Chemistry WebBook Examples

State: $3d^2E$

Energy (cm^{-1})	Med.	Transition	λ_{min} (nm)	λ_{max} (nm)	References
$T_0 = 66536$	gas	$3d^2E''-X$	144	150	Herzberg and Shoosmith, 1956 Herzberg, 1961 DiGiuseppe, Hudgens, et al., 1982

Electronic
spectra

Thermo-
chemical
data

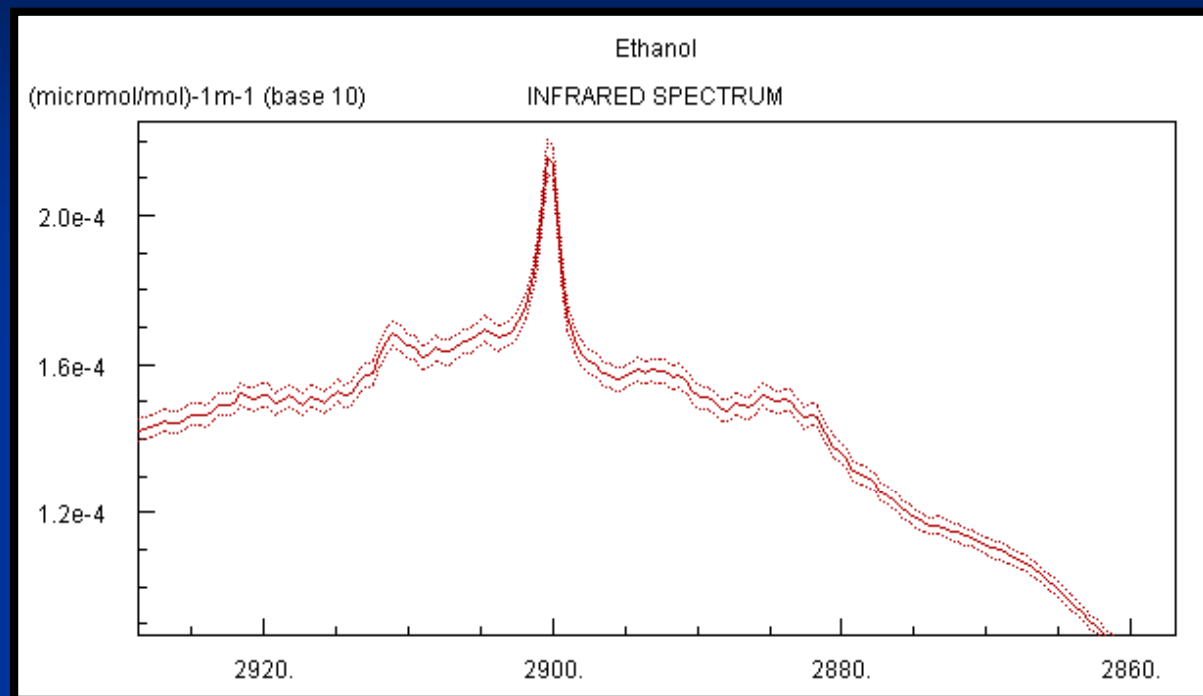
Gas phase thermochemistry data

Go To: [Top](#), [References](#), [Notes](#) / [Error Report](#)

Data compilation [copyright](#) by the U.S. Secretary of Commerce on behalf of the U.S.A. All rights reserved.

Quantity	Value	Units	Method	Reference	Comment
$\Delta_f H^\circ_{\text{gas}}$	145.69	kJ/mol	Review	Chase, 1998	Data last reviewed in June, 1969
$\Delta_f H^\circ_{\text{gas}}$	$147. \pm 1.$	kJ/mol	N/A	Tsang, 1996	
Quantity	Value	Units	Method	Reference	Comment
$S^\circ_{\text{gas,1 bar}}$	194.17	J/mol*K	Review	Chase, 1998	Data last reviewed in June, 1969

Chemistry WebBook Examples



Infrared spectra
with uncertainty

Chemical (ion)
reaction data

Appearance energy determinations

Ion	AE (eV)	Other Products	Method	Reference	Comment
$C_5H_{10}^+$	10.04 ± 0.05	H ₂ O	EI	Harnish, Holmes, et al., 1990	LL

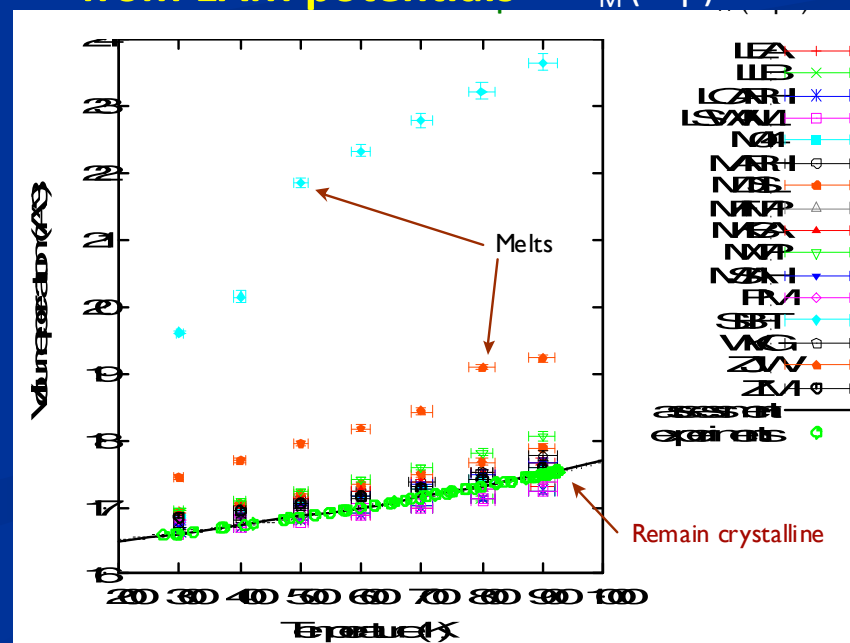
Interatomic Potentials Repository

- Accurate interatomic potentials (forcefields) from known and trusted sources are essential in molecular simulation.
- If you can't trace your file or potential to the original source, you don't really know what you have. This calls results into question and is bad for both users and developers of potentials.
- Repository: <http://www.ctcms.nist.gov/potentials/>
- **100+ element and alloy interatomic potentials are available for download.**
- submitted or vetted by their authors and referenced
- files from other users or LAMMPS can be checked against documented versions
- Recent usage: ~5500 content pages per month to ~1000 IP addresses (not crawlers)
- Current and future work:
 - test results (with appropriate reference data) for interatomic potentials on the website
 - commentaries on the strengths and weaknesses of models and data
 - error assessment beyond standard deviations
 - more potentials, including non-metallic potentials
- **Contact: Chandler Becker, cbecker@nist.gov**

Available now:

Elements	Selected multi-component systems
Ag, Al, Au, Co, Cs, Cu, Fe, K, Li, Mg, Mo, Na, Nb, Ni, Pb, Pt, Rb, Ru, Si, Ta, Ti, V, W, Zr	Ag-Cu
	Al-Cu, Al-Fe, Al-H, Al-Mg, Al-Mn-Pd, Al-Ni, Al-Pb, Al-Si-Mg-Cu-Fe, Al-Ti
	C-H-O
	Cu-Ag, Cu-Al, Cu-Fe, Cu-Ni, Cu-Pb, Cu-Ta, Cu-Zr
	Fe-Al, Fe-C, Fe-Cu, Fe-Cu-Ni, Fe-Ni, Fe-P, Fe-V
	Mg-Al
	Ni-Al, Ni-Al-H, Ni-Cu, Ni-Fe, Ni-Zr
	UO ₂ , (U,Pu,Np)O ₂

Al atomic volumes from EAM potentials $T_M(\text{exp}) = 933 \text{ K}$



Assessment: Eric Lass, et al., in preparation (2012)

CALPHAD File Repository

C.E. Campbell and U.R. Kattner, NIST
L.M. Bartolo, Kent State Univ.



■ Motivation:

- A CALPHAD assessment for a given system requires collecting all the available experimental and computational data, evaluating the data, and developing functional composition, temperature, and pressure descriptions. **A file repository will improve efficiency and reproducibility of the method.**

■ Current progress:

- Established a workspace to test repository structure
- Repository format tested with files from recently published CALPHAD assessments
- Categories used to tag data include, but are not limited to:
 - Authors and source information
 - Systems (i.e. A-B)
 - Property class (thermodynamics, diffusion, molar volume, elastic properties)
 - Phases (gas, liquid, disordered and ordered solids)
 - Types of resources (functional description files, experimental data files, macros, scripts)



Future Work:

- Implement a more user-friendly search interface
- Recruit collaborators to test structure and input work
- Define standards for phase names

carelyn.campbell@nist.gov

ursula.kattner@nist.gov

The screenshot displays the NIST/MatDL workspace interface. The main window shows a list of items with columns for Name, Date, and Version. The selected item is 'Ag-AL1-200...'. The detailed view shows the functional description file content, including references and the functional description itself. The right sidebar shows the 'Summary' tab with fields for Author (Jacques, P., Nakano, J.), Type (Functional description file), and Format (text/plain).

Similar workspace structures are being explored and developed for first-principles and experimental work.

Current Efforts Toward a General Data Repository

C.E. Campbell, U.R. Kattner, A.A. Dima, D. Foxvog

Initial focus is on phase-based data used by CALPHAD-based assessments.

- **Developing needed universal identifiers**
 - **Crystal Structure**
 - **Phase Names**
 - **Materials** (including processing history and composition)
- **Developing ontologies to describe materials data with initial emphasis on**
 - Phase equilibria
 - Thermochemistry
 - Diffusion
- **Investigating a variety of data-interchange and representation formats (e.g. JSON, BSON, XML)**
- **Developing tools to transform data for use in other modeling tools**
- **Constructing a Wiki to define terminology**

carelyn.campbell@nist.gov; ursula.kattner@nist.gov

NIST Standard Reference Simulation Website

<http://go.usa.gov/rHYm>

- **Objectives:** Provide well-documented results from molecular simulation (Monte Carlo, Molecular Dynamics) that can be treated like experimental standard reference data.

- **Examples:**

- equations of state
- phase coexistence conditions
- transport properties

- **Intended Use:**

- reference data for simulation users
- data for algorithm validation
- re-use of published data for original research

- **Maintainers:**

Vincent Shen, vincent.shen@nist.gov

Daniel Siderius, daniel.siderius@nist.gov

William Krekelberg, william.krekelberg@nist.gov

The screenshot shows the NIST Standard Reference Simulation Website page. The header includes the NIST logo and navigation links: NIST Time, NIST Home, About NIST, Contact Us, and A-Z Site Index. Below the header is the Material Measurement Laboratory logo and a navigation menu with links for About MML, Publications, Topic/Subject Areas, Products/Services, News/Multimedia, Events, Programs/Projects, and Facilities. The main content area is titled "NIST Standard Reference Simulation Website" and contains a summary, description, systems available, start and end dates, lead organizational unit, staff, and contact information. The summary states that the website is an ongoing project to provide well-documented simulation results for various systems. The description explains that molecular simulations, particularly Monte Carlo Molecular Simulation and Molecular Dynamics Simulation, are used to compute properties of systems. The systems available include Lennard-Jones, Stockmayer, Ethane, n-Octane, SPC/E Water, and Hard-Sphere Fluid. The contact information lists Vincent Shen, Daniel Siderius, and William Krekelberg.

NIST Time | NIST Home | About NIST | Contact Us | A-Z Site Index

Material Measurement Laboratory

About MML | Publications | Topic/Subject Areas | Products/Services | News/Multimedia | Events | Programs/Projects | Facilities

NIST Home > MML > Chemical and Biochemical Reference Data Division > Computational Chemistry Group > NIST Standard Reference Simulation Website

Select Language * | SHARE | Powered by Google Translate

NIST Standard Reference Simulation Website

Summary:
The Standard Reference Simulation Website is an ongoing project whose aim is to provide well-documented simulation results for a variety of systems and from various simulation techniques. The results contained here are usually generated in-house at NIST but, when certain criteria are satisfied, may also include results from provided from outside collaborators.

Description:
Molecular simulations, in particular Monte Carlo Molecular Simulation and Molecular Dynamics Simulation, are methods for computing the properties of some kind of system, for which the intermolecular interactions are specified, via mathematical relationships derived from statistical mechanics. Since statistical mechanics itself makes no reference to molecular simulation of any kind, the properties that derive from statistical mechanics should not depend on the particular simulation algorithm used to compute properties for a specified model. Consequently, the results obtained from a molecular simulation can be thought of as characteristic of the model system, subject only to statistical uncertainty in those results, if the simulation technique follows necessary rules (e.g., detailed balance or microscopic reversibility, depending on the particular algorithm) and is computationally robust. Our goal in this project is to publish well-documented simulation results for reliable and well-vetted simulation software for a variety of systems, many of which are commonly used in molecular simulations, that can be treated similar to "standard reference data" that is generated in an laboratory setting. The data contained here may be used to validate and test new or existing molecular simulation software, as reference data, or for other appropriate applications. Most of the results contained here are generated in-house at NIST, but we will also include results from collaborators provided certain criteria are satisfied (see "Criteria..." below). In addition, it is our goal to provide data from molecular simulations in a raw or unprocessed format, when possible, so that the data may be reprocessed according to end users' particular needs. To that end, we also provide some software that may be used to reprocess data contained here.

Systems Available:

- Lennard-Jones
- Stockmayer
- Ethane
- n-Octane
- SPC/E Water
- Hard-Sphere Fluid

Start Date:
August 1, 2006

End Date:
Ongoing

Lead Organizational Unit:
MML

Staff:
Vincent Shen
William Krekelberg
Daniel Siderius
Raymond Mountain

Associated Products:
NIST Standard Reference Database 173

Contact

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Email: vincent.shen@nist.gov
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Fax: 301-975-2510

Daniel Siderius
Email: daniel.siderius@nist.gov
Phone: 301-975-5968
Fax: 301-869-4020

Selected Practice Guides in Materials Sciences

NIST
National Institute of
Standards and Technology
U.S. Department of Commerce

MATERIAL MEASUREMENT LABORATORY

Selected NIST-Recommended Practice Guides in Material Sciences

Courtesy of
SRD 31, Phase Equilibria Diagrams Database
<http://www.nist.gov/srd/nist31.cfm>
SRD 84, Inorganic Crystal Structure Database
<http://www.nist.gov/srd/nist84.cfm>

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General Discussion of Phase Diagrams
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*Ajit Jilavenkatesa, Stanley J Dapkunas
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The Fundamentals of Neutron Powder Diffraction
John RD Copley (NIST SP 960-2)

**The Use of Nomenclature in Dispersion
Science and Technology,**
Vincent A Hackley and Chiara F Ferraris (NIST SP 960-3)

**Rockwell Hardness Measurement of Metallic
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**Capacitance Cell Measurement of the
Out-of-Plane Expansion of Thin Films**
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Test Procedures for Developing Solder Data
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Stanley J Dapkunas (NIST SP 960-9)

X-Ray Topography
David R Black and Gabrielle G Long (NIST SP 960-10)

**Data Evaluation Theory and Practice
for Materials Properties**
Ronald G Munro (NIST SP 960-11)

**Pore Characterization in Low-k Dielectric Films
Using X-Ray Reflectivity: X-Ray Porosimetry**
*Christopher L Soles, Hae-Jeong Lee, Eric K Lin,
and Wen-Ji Wu (NIST SP 960-13)*

**DTA and Heat-Flux DSC Measurements
of Alloy Melting and Freezing**
*WJ Boettinger, UR Kottner, K-W Moon
and JH Perepezko (NIST SP 960-15)*

Fractography of Ceramics and Glasses
George D Quinn (NIST SP 960-16, with errata)

**Porosity and Specific Surface Area
Measurements for Solid Materials**
*Peter Klöbes, Klaus Meyer and
Ronald G Munro (NIST SP 960-17)*

**Computing Uncertainty for Charpy Impact Machine
Test Results**
*JD Splett, CN McCowan, HK Iyer
and C-M Wang (NIST SP 960-18)*

Measurement Issues in Single-Wall Carbon Nanotubes
*Stephen Freiman, Stephanie Hooker, Kalman Migler
and Sivaram Arepalli (NIST SP 960-19)*

For a complete list of Practice Guides visit:
http://www.nist.gov/public_affairs/factsheet/practiceguides.cfm

Available Party Favors

- Demo CDROMs – Phase Equil. Diagrams (*SRD 31*)
- Demo CDROMs – ICSD (Inorg. Crystal Structures) (*SRD 84*)
- CDROMs - Selected Practice Guides

- ***Also:*** laptop available running full versions of SRD 31 and SRD 84