

Chapter 5 Examples of Use

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	Composition (System)/ Property → Multiple regression equation	Composition → Property prediction	Composition (System)/ Property → Composition optimization
Multiple regression equation (linear equation) With additivity	3.1	3.2 3.4	3.3 3.6 (2 properties)
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Notes

- 1) Parts where some operation or checking is necessary are encircled with the following colors in each window.

Selection or input	:	
Operation of button or icon	:	
Checking	:	

- 2) Refer the User's Manual for detailed operation. Necessary chapters and sections are indicated under each example's title.
- 3) Number of searched data (Total Number) and data content in the [Data List of Property or Structure] window are different depending on the Version of INTERGLAD. So when the user tries the same example, the Total Number and the content may be different from those of the example described here. Ver.7.1.3.2.01–7.2.1.0.05 of INTERGLAD are used in these examples.

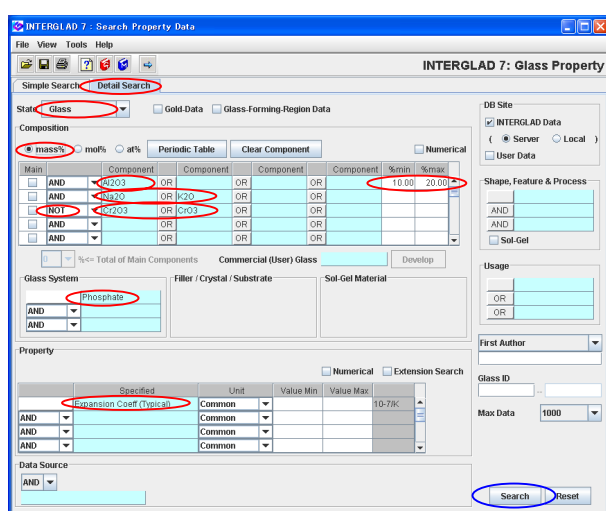
1. Search and Analysis of Property Data

1.1 Search with a complicated composition – Thermal expansion coefficient of phosphate glasses

Search thermal expansion coefficient data of phosphate glasses with 10-20 mass% of Al_2O_3 , containing Na_2O or K_2O , and not containing Cr Oxides.

<Refer to B of Chapter 3 and 2 of Chapter 4>

- 1) Specification of search conditions ([Search Property Data] window with [Detail Search] tag)
→ Search



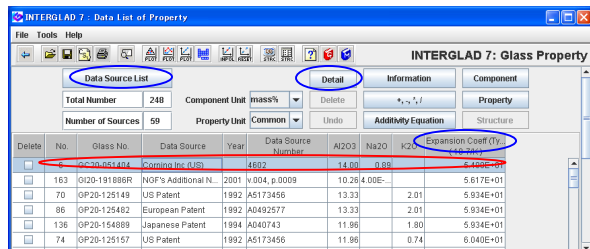
- Choose 'mass%' for the unit of composition. The default of the unit is mol%.
- Select 'Na2O' and 'K2O' in the same row with connection of 'OR.' In this case simultaneous selection is not available on the periodic table.
- Cr Oxides can be selected by selecting 'Cr' and 'O' on the Periodic Table.
- The order of selection for search conditions is free.
- More the search conditions become complex, longer the search time.
- 'Expansion Coeff (Typical)' is selected for the [Specified] of the [Property] columns. The selection of 'Linear Expansion Coeff' (a middle category item, boldtype) brings the same result.

- 2) Search result ([Data List of Property] window)

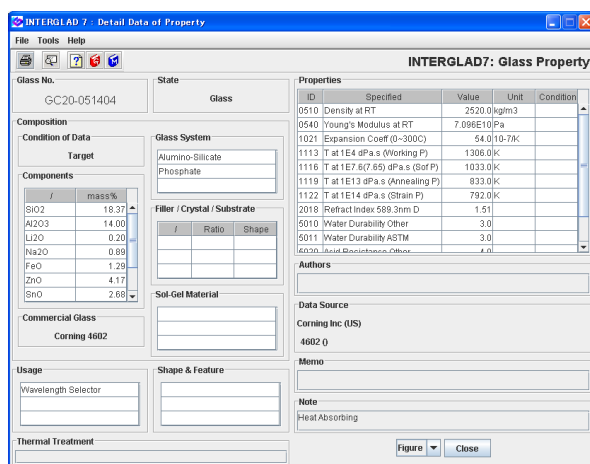
No.	Glass No.	Data Source	Year	Data Source Number	Al2O3	Na2O	K2O	Expansion Coeff (Typical)
1	GP20-035418	Japanese Patent	1986	A036137	12.16	4.22		6.86E+01
2	GP20-037218	Japanese Patent	1983	A128941	15.00	5.50		1.29E+02
3	GP20-045104	J. Am. Ceram. Soc.	1981	v084, p.0208	16.00		2.25	7.44E+01
4	GP20-045105	J. Am. Ceram. Soc.	1981	v084, p.0208	17.22		4.34	6.67E+01
5	GP20-045284	J. Am. Ceram. Soc.	1985	v001, p.0007	17.03		4.29	6.70E+01
6	GP20-051404	Corning Inc. (US)	1987	A454497	14.00	0.89		5.40E+01
7	GP20-065115	Japanese Patent	1987	A235231	11.21		8.22	9.80E+01
8	GP20-065117	Japanese Patent	1987	A235231	11.71		13.70	1.07E+02
9	GP20-065120	Japanese Patent	1987	A235231	10.93		15.53	1.05E+02
10	GP20-065121	Japanese Patent	1987	A235231	10.02	1.10	12.17	1.18E+02
11	GP20-065122	Japanese Patent	1987	A235231	10.13	3.33	8.94	1.08E+02
12	GP20-065123	Japanese Patent	1987	A235231	10.06		8.88	1.23E+02
13	GP20-065124	Japanese Patent	1987	A235231	11.83	1.02	7.44	1.09E+02
14	GP20-065125	Japanese Patent	1987	A235231	11.80	1.02	7.42	1.09E+02
15	GP20-067932	Japanese Patent	1981	A051574	10.00		5.00	9.80E+01
16	GP20-067938	Japanese Patent	1981	A051574	10.00		5.00	8.30E+01
17	GB20-087441	Glass Hand Book (J)	1975	v001, p.0136	17.00	18.00	11.00	1.55E+02
18	GP20-094216	US Patent	1985	A454497	2.05	15.38		1.25E+02
19	GP20-094218	US Patent	1985	A454497	41	15.60		1.20E+02
20	GP20-102250	Japanese Patent	1989	A242440	13.00		1.00	6.70E+01
21	GP20-102251	Japanese Patent	1989	A242440	16.00		2.20	6.90E+01
22	GP20-102253	Japanese Patent	1989	A242440	16.00		20	6.40E+01

- Take notice of 'Total Number' of the Data Source.
- A table with values of components, property data etc., which are specified as the search conditions, appears.
- If necessary, analyze the dataset using Ternary Plot or XY Plot.

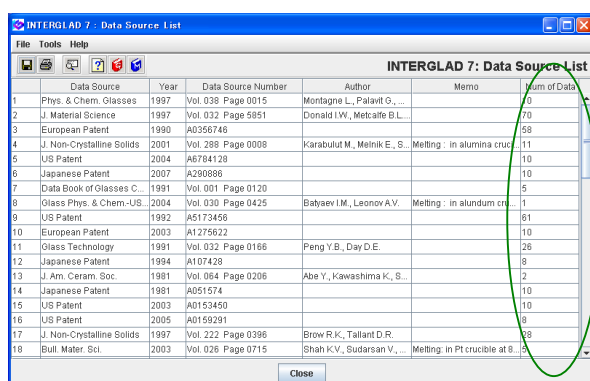
3) Utilization of the search result ([Detail Data of Property] window and [Data Source List] window)



- Sorting of each column is available. Click an item label holding down the Ctrl key.
- In this example, by sorting 'Expansion Coeff' the glass with the lowest value can be found. The detailed data of the glass is checked by selecting its row and clicking the [Detail] button.



[Detail Data of Property] window



[Data Source List] window

- The [Data Source List] window opens by clicking the [Data Source List] button in the [Data List of Property] window.
- Number of glasses of each data source is shown in the [Num of Data] column.

1.2 Search under complicated conditions on composition and property – Search for non-alkali glasses with a specified strain point

Search non-alkali glasses with strain point $600 \pm 30^\circ\text{C}$ (content of alkali oxides ≤ 0.5 mass%, data sources except patents).

<Refer to B of Chapter 3 and 2 of Chapter 4>

- 1) Specification of search conditions ([Search Property Data] window with [Detail Search] tag)
→ Search

- Select 'Glass General' for the State. Glass General includes Glass-Ceramics, Modified Glass, etc.
- Select italic 'R2O', by which all glasses containing alkali components are searched.
- Input 0.5 for the [%max] cell as the maximum content of R2O. When in the [%min] cell 0 is inputted, or none inputted, glasses not containing alkali oxides are also searched.
- Strain point has 2 IDs with different viscosity values. This example connects 2 IDs with OR. If necessary, select an ID. To select a property item, select using a keyword is convenient.

- 2) Search result ([Data List of Property] window)

Delete	No.	Glass No.	Data Source	Year	Data Source Number	Na2O	K2O	R2O	T at 1E14 dPa.s (Str. (C))	T at 1E14.5 dPa.s (C)
	1	0B09-010267	Handbook of Glass Pr.	1980	v.001, p.0248					
	2	MC05-051260	Schott AG (DE)		AF-45				6.270E+02	6.280E+02
	3	OC05-051368	Corning Inc (US)	1976	1415				6.200E+02	
	4	OC05-051408	Corning Inc (US)	1981	8700				5.750E+02	
	5	OC03-051416	Corning Inc (US)	2003	7059		0.30		5.930E+02	
	6	OC05-051488	Corning Inc (US)		8410				5.930E+02	
	7	OC40-051489	Corning Inc (US)		8445				6.230E+02	
	8	OC05-051915	Hoya Corp (J)		NA-45					6.100E+02
	9	OC06-051918	Hoya Corp (J)	1989	LE-30					6.250E+02
	10	OC03-052344	Nitto Boseki (J)		NIITBOE-GLAS			0.50	6.100E+02	
	11	GU05-056013	J. Am. Ceram. Soc.	1975	v.058, p.0300				5.870E+02	
	12	OC03-066057	Hoya Corp (J)		BaCD5-589-613					6.000E+02
	13	OC03-066069	Hoya Corp (J)		BaCD18-638-555					6.050E+02
	14	OC05-066091	Hoya Corp (J)		LaC9-691-547					6.170E+02
	15	OC05-066092	Hoya Corp (J)		LaC10-720-503					6.110E+02
	16	OC05-066094	Hoya Corp (J)		LaC12-678-555					6.240E+02
	17	OC05-066095	Hoya Corp (J)		LaC13-694-533					6.300E+02
	18	SB09-070436	Handbook of Glass D.	1982	v.00A, p.0589					6.280E+02
	19	OC03-078651	J. Non-Crystalline Sol.	1986	v.080, p.0141					6.280E+02
	20	OC03-086665	Schott Glas (Jena) (DE)		D187					6.150E+02
	21	OC03-086666	Schott Glas (Jena) (DE)		D188					6.100E+02
	22	OC03-086667	Schott Glas (Jena) (DE)		D189					6.200E+02
	23	OC03-086668	Schott Glas (Jena) (DE)		D263					6.150E+02

- 74 glasses are listed as the search result.
- All the alkali oxide components contained in the listed glasses are shown in the table. 'R2O' with the normal style means alkali oxides written as R₂O in data sources.

3) Utilization of the search result

INTERGLAD 7: Data List of Property

File Tools Help

INTERGLAD 7: Glass Property

Data Source List

Total Number: 74

Component Unit: mass%

Property Unit: Common

Number of Sources: 63

Buttons: Detail, Information, Component, Property

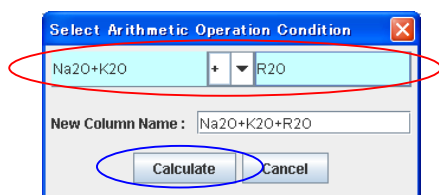
Buttons: Add, Subtract, Multiply, Divide, Additivity Equation

Delete	No.	Glass No.	Data Source	Year	Data Source Number	Na ₂ O+K ₂ O+R ₂ O	T at 1E14 dPa.s (St. (C))	T at 1E14.5 dPa.s (C)	Na ₂
☐	5	OC03-051416	Corning Inc (US)	2003	7059	0.30	5.930E+02		0
☐	58	OB03-174769	Data Book of Glass...	1991	v.001, p.0134	0.40		6.200E+02	0
☐	10	OC03-052344	Nitto Boseki (J)		NITTOBOE-GLASS	0.50	6.100E+02		
☐	1	OB09-010267	Handbook of Glass...	1986	v.001, p.0246			6.260E+02	
☐	2	MC05-051260	Schott AG (DE)		AF-45		6.270E+02		
☐	3	OC05-051368	Corning Inc (US)	1976	1415		6.200E+02		
☐	4	OC05-051408	Corning Inc (US)	1981	6700		5.750E+02		
☐	6	OC05-051498	Corning Inc (US)		9410		5.930E+02		
☐	7	OC09-051489	Corning Inc (US)		9445		6.230E+02		
☐	8	OC05-051915	Hoya Corp (J)		NA-45			6.100E+02	
☐	9	OC06-051918	Hoya Corp (J)	1989	LE-30			6.290E+02	
☐	11	OC05-056013	J. Am. Ceram. Soc.	1975	v.058, p.0300		5.870E+02		
☐	12	OC03-066057	Hoya Corp (J)		BaCD5-599-610			6.000E+02	
☐	13	OC03-066069	Hoya Corp (J)		BaCD18-638-555			6.050E+02	
☐	14	OC05-066091	Hoya Corp (J)		LaC9-691-547			6.170E+02	
☐	15	OC05-066092	Hoya Corp (J)		LaC10-728-503			6.110E+02	
☐	16	OC05-066094	Hoya Corp (J)		LaC12-678-555			6.240E+02	
☐	17	OC05-066095	Hoya Corp (J)		LaC13-694-533			6.300E+02	
☐	18	OB09-078435	Handbook of Glass...	1983	v.00A, p.0586			6.260E+02	
☐	19	OC03-079851	J. Non-Crystalline S...	1986	v.080, p.0141			6.290E+02	
☐	20	OC03-088685	Schott Glas (Jena) (C...		D187			6.150E+02	
☐	21	OC03-088686	Schott Glas (Jena) (C...		D188			6.100E+02	

- Sum values of alkali content in each glass can be calculated and listed in ascending order. Using the [Arithmetic Operation] button, first calculate Na₂O+K₂O, then calculate (Na₂O+K₂O)+R₂O, and sort.

<Refer 2.2 (2) (C) 10) of Chapter 4>

- Most of composition data are unknown due to catalogue data.



[Arithmetic Operation] dialog box

4) Detailed data ([Detail Data of Property] window)

INTERGLAD 7: Detail Data of Property

File Tools Help

INTERGLAD 7: Glass Property

Glass No.: GC03-051416

State: Glass

Properties

ID	Specified	Value	Unit	Condition
0050	Shear Modulus	2.617E10	Pa	
0060	Poisson Ratio	0.25		
0160	Fracture Toughness	0.8	MPa.m ^{1/2}	
0215	Stress Corrosion Resist	18.4		stress c...
0510	Density at RT	2753.0	kg/m ³	
0540	Young's Modulus at RT	6890.0	kgf/mm ²	
1021	Expansion Coeff (0-200C)	46.6	10 ⁻⁶ /K	
1113	T at 1E4 dPa.s (Working P)	1433.0	K	
1116	T at 1E7.6(7.65) dPa.s (Sof P)	1117.0	K	
1119	T at 1E13 dPa.s (Annealing P)	912.0	K	
1123	T at 1E14.5 dPa.s (Structure D)	668.0	K	

Authors:

Data Source: Corning Inc (US) 7059 (2003)

Memo:

Note: Fusion Glass Substrate

Buttons: Figure, Close

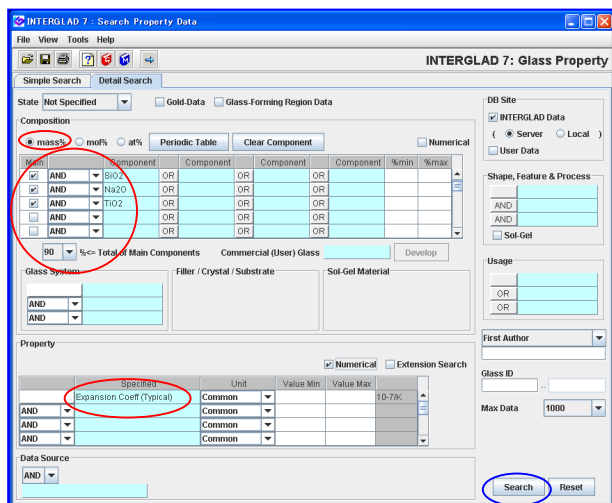
- Detailed data of a glass can be checked in the [Detail Data of Property] window from the [Detail] button after selecting a glass row.

1.3 Ternary plot analysis of property data – Thermal expansion coefficient of $\text{SiO}_2\text{-TiO}_2\text{-Na}_2\text{O}$ glasses

Investigate relation between composition and thermal expansion coefficient on $\text{SiO}_2\text{-TiO}_2\text{-Na}_2\text{O}$ glasses. <Refer to B and C.1 of Chapter 3, and 2 and 3.1 of Chapter 4>

1) Specification of search conditions ([Search Property Data] window with [Detail Search] tag)

→ Search



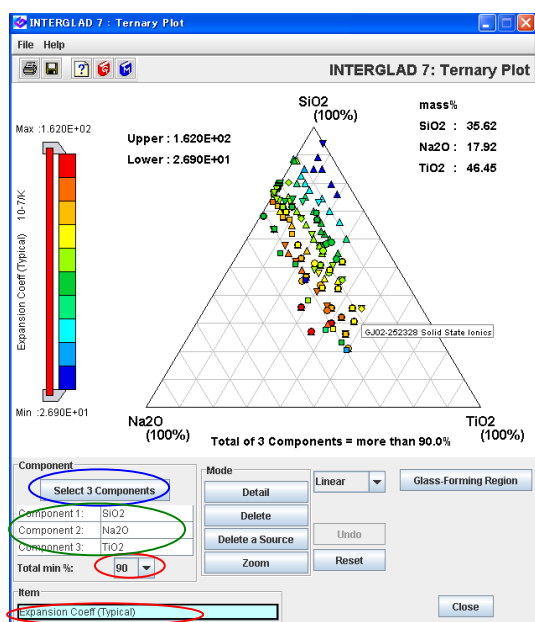
- Choose '90' mass% as the minimum Total of Main Components, SiO_2 , TiO_2 and Na_2O .
- Select 'Expansion Coeff (Typical)' for the Specified of the Property.

2) Search result ([Data List of Property] window)

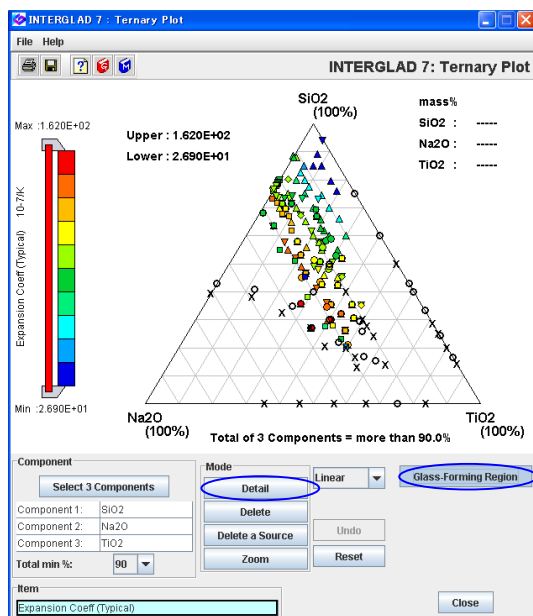
No.	Glass No.	Data Source	Year	Data Source Number	SiO ₂	Na ₂ O	TiO ₂	Expansion Coeff (Typical) (10 ⁻⁷ /K)
1	0B02-006032	Handbook of Glass.	1986	v.001, p.0163	67.09	15.21	17.71	8.400E+01
2	0B02-006033	Handbook of Glass.	1986	v.001, p.0163	51.85	15.56	32.59	1.100E+02
3	0B02-006034	Handbook of Glass.	1986	v.001, p.0163	49.04	20.56	30.40	1.120E+02
4	0B02-006035	Handbook of Glass.	1986	v.001, p.0163	35.58	20.57	43.87	1.080E+02
5	0B02-006036	Handbook of Glass.	1986	v.001, p.0163	42.29	21.44	36.27	1.160E+02
6	0B02-006037	Handbook of Glass.	1986	v.001, p.0163	69.61	23.38	6.99	1.100E+02
7	0B02-006038	Handbook of Glass.	1986	v.001, p.0163	50.68	22.51	26.81	1.070E+02
8	0B02-006039	Handbook of Glass.	1986	v.001, p.0163	30.71	22.63	46.66	1.150E+02
9	0B02-006040	Handbook of Glass.	1986	v.001, p.0163	58.00	25.69	16.31	1.180E+02
10	0B02-006041	Handbook of Glass.	1986	v.001, p.0163	42.61	26.03	31.36	1.160E+02
11	0B02-006042	Handbook of Glass.	1986	v.001, p.0163	53.26	26.93	19.80	1.270E+02

- 200 glasses are searched.

3) Ternary plot

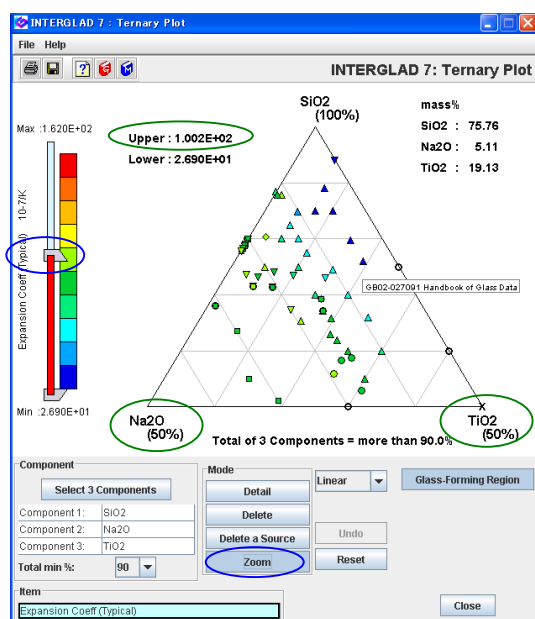


- Open the [Ternary Plot] window by clicking the [Ternary Plot] icon. Select SiO_2 , TiO_2 and Na_2O as 3 Components, '90' for the Total min%, and 'Expansion Coeff (Typical)' for the Item.
- Value levels of thermal expansion coefficients can be overviewed by plot-points with ten steps of colors in the diagram. Thermal expansion coefficient is high in the



center region and decreases as the position moves to the upper right (near to SiO₂ 100%).

- The Glass No. and Data Source of each plot-point are indicated in a balloon by putting the mouse-pointer at a plot-point. The detailed data of each plot-point can be checked by clicking a plot-point with the [Detail] button active.
- The Glass-forming region data are shown by clicking the [Glass-Forming Region] button. The boundary line is assumed to be between marks of ○(Glass) and ×(Non-Vitrified).
- Glass-forming region data in the database are those of glasses in which total of 3 components is 100%. Note that in the collected data of this example total of 3 components is 90-100%.
- The state (glass or non-vitrified) of each plot-point can be checked by opening each [Detail Data of Property] window.
- The detailed data of glass-forming region also can be checked by clicking a mark or line with the [Detail] button active.



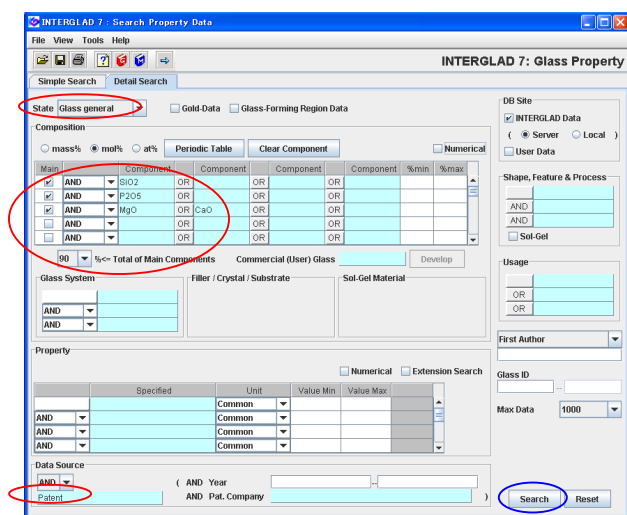
- By sliding the slider, property value range of glasses in the diagram can be changed. In the example of the left figure thermal expansion coefficient is limited to $\leq 100 \times 10^{-7}/K$, and the ternary diagram with SiO₂ (100%), Na₂O (50%), TiO₂ (50%) is shown by using the [Zoom] button.

1.4 Ternary plot analysis of pseudo-ternary system – Patent investigation of $\text{SiO}_2\text{-P}_2\text{O}_5\text{-(MgO+CaO)}$ glass system

Show a ternary plot of $\text{SiO}_2\text{-P}_2\text{O}_5\text{-(MgO+CaO)}$ pseudo-ternary system for patent investigation.

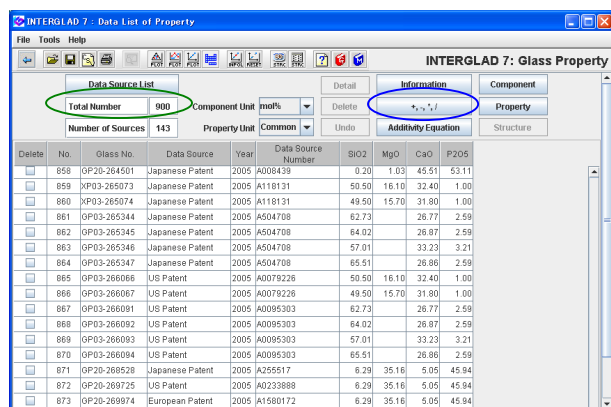
<Refer to B and C.1 of Chapter 3, and 2 and 3.1 of Chapter 4>

- 1) Specification of search conditions ([Search Property Data] window with [Detail Search] tag
→ Search

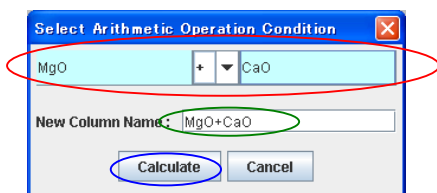


- Select 'Glass General' for the State.
- Select 'MgO' and 'CaO' in the same row with OR connection.
- Specify 90% as the minimum value for the Total of Main Components. Check the [Numerical] checkbox to search only numerical data.
- Select 'Patent' for the Data Source.

- 2) Search result ([Data List of Property] window)



- 900 glasses are listed.
- When 'MgO+CaO' is specified and calculated in the [Arithmetic Operation] dialog box after clicking the [+ , -, *, /] button, the calculated values are listed.



[Arithmetic Operation] dialog box

INTERGLAD 7 : Data List of Property

File Tools Help

INTERGLAD 7: Glass Property

Data Source List

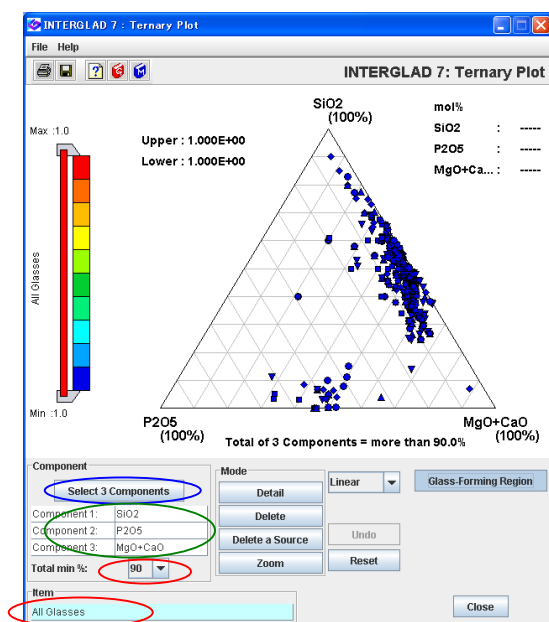
Total Number: 900
Number of Sources: 143

Component Unit: mol%
Property Unit: Common

Buttons: Detail, Information, Component, Delete, Additivity Equation, Property, Structure, Undo

Delete	No.	Glass No.	Data Source	Year	Data Source Number	MgO+CaO	SiO ₂	MgO	CaO	P ₂ O ₅
☐	858	OP03-264501	Japanese Patent	2005	A008439	46.54	0.2	1.03	45.51	63.11
☐	859	XP03-265073	Japanese Patent	2005	A118131	48.50	50.50	16.10	32.40	1.00
☐	860	XP03-265074	Japanese Patent	2005	A118131	47.50	49.50	15.70	31.80	1.00
☐	861	OP03-265344	Japanese Patent	2005	A504708	26.77	62.73		26.77	2.59
☐	862	OP03-265345	Japanese Patent	2005	A504708	26.87	64.02		26.87	2.59
☐	863	OP03-265346	Japanese Patent	2005	A504708	33.23	57.01		33.23	3.21
☐	864	OP03-265347	Japanese Patent	2005	A504708	26.86	65.51		26.86	2.59
☐	865	OP03-266066	US Patent	2005	A0079226	48.50	50.50	1.10	32.40	1.00
☐	866	OP03-266067	US Patent	2005	A0079226	47.50	49.50	1.70	31.80	1.00
☐	867	OP03-266091	US Patent	2005	A0085303	26.77	62.73		26.77	2.59
☐	868	OP03-266092	US Patent	2005	A0085303	26.87	64.02		26.87	2.59
☐	869	OP03-266093	US Patent	2005	A0085303	33.23	57.01		33.23	3.21
☐	870	OP03-266094	US Patent	2005	A0085303	26.86	65.51		26.86	2.59
☐	871	OP20-269528	Japanese Patent	2005	A355617	40.21	6.29	35.16	5.05	45.94
☐	872	OP20-269725	US Patent	2005	A0233888	40.21	6.29	35.16	5.05	45.94
☐	873	OP20-269974	European Patent	2005	A1580172	40.21	6.29	35.16	5.05	45.94

3) Ternary Plot



- Open the [Ternary Plot] window by clicking the [Ternary Plot] icon. Select SiO₂, P₂O₅, (MgO+CaO) for the 3 Components, 90% for the Total min, and 'All Glasses' for the Item. (The Default is All Glasses)
- A Ternary Plot of SiO₂-P₂O₅-(MgO+CaO) pseudo-ternary system appears. Compositions of registered patents are visualized. This result does not include data of the binary systems, SiO₂-P₂O₅, P₂O₅-(MgO+CaO), and (MgO+CaO)-SiO₂, because the search is conducted under the condition that the 3 components including a component 'MgO or CaO' are necessary.

1.5 XY plot analysis of properties – Refractive index vs. Abbe value

Investigate a relation between refractive index and Abbe value of glasses.

<Refer to B and C.2 of Chapter 3, and 2 and 3.2 of Chapter 4>

- 1) Specification of search conditions ([Search Property Data] window with [Detail Search] tag
→ Search

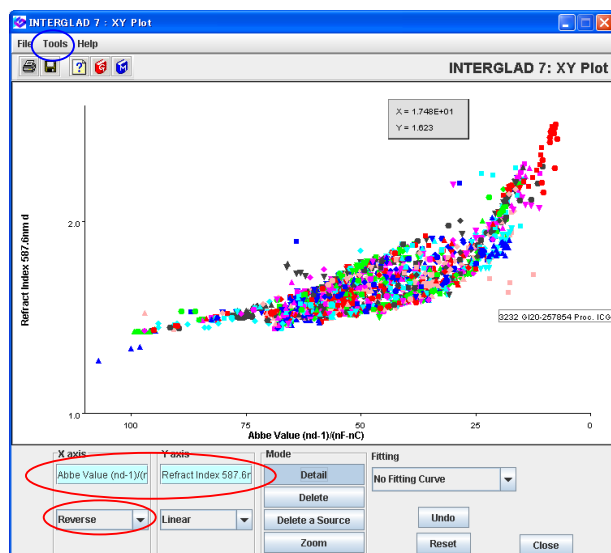
- Select 'Glass' for the State.
- As for refractive index, data measured by illuminants with various wavelengths are in the database. In this example, data by He d-line with 587.6nm are searched.
- Select '(nd-1)/(nF-nC)' for the Abbe value.
- Check in the [Numerical] checkbox.
- Select 'NOT Patent' for the Data Source.

- 2) Search result ([Data List of Property] window)

No.	Glass No.	Data Source	Year	Data Source Number	Refract Index 587.6	Abbe Value (nd-1)/(nF-nC)
1	0J05-00826	Olafsch. Ber.	1987	v.060, p.0234	1.502	6.560E+01
2	0J05-00827	Olafsch. Ber.	1987	v.060, p.0234	1.502	6.620E+01
3	0J05-00828	Olafsch. Ber.	1987	v.060, p.0234	1.502	6.660E+01
4	0J05-00829	Olafsch. Ber.	1987	v.060, p.0234	1.502	6.665E+01
5	0J05-00830	Olafsch. Ber.	1987	v.060, p.0234	1.503	6.670E+01
6	0J05-00831	Olafsch. Ber.	1987	v.060, p.0234	1.503	6.658E+01
7	0J05-00832	Olafsch. Ber.	1987	v.060, p.0234	1.504	6.688E+01
8	0J05-00833	Olafsch. Ber.	1987	v.060, p.0234	1.504	6.722E+01
9	0J05-00834	Olafsch. Ber.	1987	v.060, p.0234	1.503	6.723E+01
10	0J01-014872	J. Ceram. Soc. Japan	1985	v.093, p.0490	1.462	6.750E+01
11	0B03-017328	Handbook of Glass.	1987	v.00C, p.0910	1.611	5.350E+01
12	0B03-017330	Handbook of Glass.	1987	v.00C, p.0910	1.621	5.320E+01
13	0B03-017331	Handbook of Glass.	1987	v.00C, p.0910	1.637	5.230E+01
14	0B03-017332	Handbook of Glass.	1987	v.00C, p.0910	1.644	5.190E+01
15	0B03-017333	Handbook of Glass.	1987	v.00C, p.0910	1.663	5.030E+01
16	0B03-017334	Handbook of Glass.	1987	v.00C, p.0910	1.661	5.100E+01

- 3302 glasses are listed.

- 3) XY Plot Analysis ([XY Plot] window)



- From the [XY Plot] icon, an XY plot (Abbe value vs. refractive index) is shown. The distribution of Abbe values and refractive indexes of 3302 glasses is visualized.
- In this example, the style of x-axis for Abbe value is set to 'Reverse', and the ranges and scales are changed from the [Tools/ Option] menu.

1.6 Search using data interpolation for high temperature properties – Viscosity at high temperatures of boro-silicate glasses

Search viscosity data at 700°C of boro-silicate glasses using data interpolation or extrapolation.

<Refer to B and C.3 of Chapter 3, and 2 and 3.3 of Chapter 4>

- 1) Specification of search conditions ([Search Property Data] window with [Detail Search] tag
→ Search

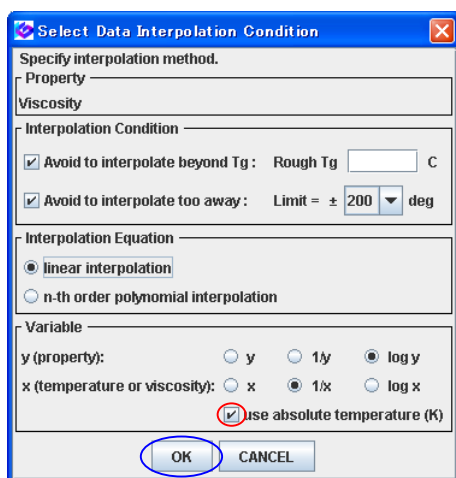
- Select 'Boro-Silicate' for the Glass System.
- Select 'Viscosity 700C' for the Property, and check in the [Extension Search] checkbox shown in the window example.
- Search of viscosity data at 700C can be performed, also when the user selects the bold type item 'Viscosity(100-1000C).' In this case data in a wide temperature range 100-1000°C are searched.

- 2) Search result ([Data List of Property] window)

Delete	No.	Glass No.	Data Source	Year	Data Source Number	Viscosity at 700C (dPa.s)
☐	1	GJ02-000026	Glastech. Ber.	1983	v.056, p.0125	
☐	2	GB04-004679	Handbook of Glass.	1986	v.001, p.0299	
☐	3	GB04-004680	Handbook of Glass.	1986	v.001, p.0299	
☐	4	GB04-004681	Handbook of Glass.	1986	v.001, p.0299	
☐	5	GB04-004682	Handbook of Glass.	1986	v.001, p.0299	
☐	6	GB04-004683	Handbook of Glass.	1986	v.001, p.0299	
☐	7	GB04-004684	Handbook of Glass.	1986	v.001, p.0299	
☐	8	GJ05-005435	J. Am. Ceram. Soc.	1980	v.063, p.0126	
☐	9	GJ05-010089	J. Am. Ceram. Soc.	1974	v.057, p.0109	
☐	10	GJ05-010070	J. Am. Ceram. Soc.	1974	v.057, p.0109	
☐	11	GB05-010245	Handbook of Glass.	1986	v.001, p.0243	
☐	12	GB05-010246	Handbook of Glass.	1986	v.001, p.0243	
☐	13	GB05-010247	Handbook of Glass.	1986	v.001, p.0243	
☐	14	GB05-010248	Handbook of Glass.	1986	v.001, p.0243	
☐	15	GB05-010249	Handbook of Glass.	1986	v.001, p.0244	
☐	16	GB05-010250	Handbook of Glass.	1986	v.001, p.0244	
☐	17	GB05-010253	Handbook of Glass.	1986	v.001, p.0244	
☐	18	GB05-010254	Handbook of Glass.	1986	v.001, p.0244	
☐	19	GB05-010255	Handbook of Glass.	1986	v.001, p.0244	
☐	20	GB05-010256	Handbook of Glass.	1986	v.001, p.0244	
☐	21	GB05-010257	Handbook of Glass.	1986	v.001, p.0244	
☐	22	GB05-010259	Handbook of Glass.	1986	v.001, p.0244	
☐	23	GB05-010260	Handbook of Glass.	1986	v.001, p.0244	

- As the search result, all the boro-silicate glasses which have registered viscosity data at high temperatures are listed. 868 glasses appear.
- When the search is performed using a keyword 'Viscosity (100-1000C),' all the glasses which have one or more data of viscosity at 100-1000°C are listed. In this case 489 glasses appear.

3) Data interpolation or extrapolation

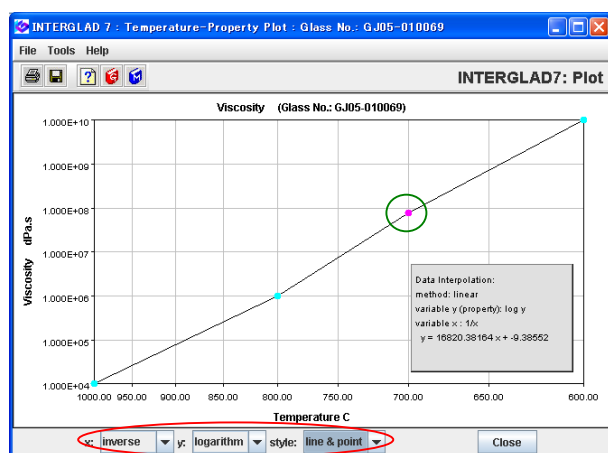


- Set conditions in the [Data Interpolation Condition] dialog box, which is opened by clicking the [Data Interpolation] icon. In this example the default of variable y (viscosity) is logy, and that of variable x (temperature) is 1/x. Check the [use absolute temperature (K)] checkbox. Then click the [OK] button.

No.	Glass No.	Data Source	Year	Data Source Number	Viscosity at 700C (dPa.s)
1	GJ02-000026	Glastech. Bar.	1982	v.056, p.0125	
2	GB04-004679	Handbook of Glass.	1986	v.001, p.0299	
3	GB04-004680	Handbook of Glass.	1986	v.001, p.0299	2.692E+01
4	GB04-004681	Handbook of Glass.	1986	v.001, p.0299	1.0E+01
5	GB04-004682	Handbook of Glass.	1986	v.001, p.0299	
6	GB04-004683	Handbook of Glass.	1986	v.001, p.0299	1.167E+03
7	GB04-004684	Handbook of Glass.	1986	v.001, p.0299	
8	GJ05-005435	J. Am. Ceram. Soc.	1980	v.063, p.0126	2.0E+10
9	GJ05-010069	J. Am. Ceram. Soc.	1974	v.057, p.0109	7.97E+07
10	GJ05-010070	J. Am. Ceram. Soc.	1974	v.057, p.0109	7.31E+09
11	GB05-010245	Handbook of Glass.	1986	v.001, p.0243	
12	GB05-010246	Handbook of Glass.	1986	v.001, p.0243	
13	GB05-010247	Handbook of Glass.	1986	v.001, p.0243	
14	GB05-010248	Handbook of Glass.	1986	v.001, p.0243	
15	GB05-010249	Handbook of Glass.	1986	v.001, p.0244	1.622E+03
16	GB05-010250	Handbook of Glass.	1986	v.001, p.0244	1.005E+03
17	GB05-010253	Handbook of Glass.	1986	v.001, p.0244	3.162E+03
18	GB05-010254	Handbook of Glass.	1986	v.001, p.0244	
19	GB05-010255	Handbook of Glass.	1986	v.001, p.0244	1.514E+04
20	GB05-010256	Handbook of Glass.	1986	v.001, p.0244	
21	GB05-010257	Handbook of Glass.	1986	v.001, p.0244	2.188E+05
22	GB05-010259	Handbook of Glass.	1986	v.001, p.0244	2.754E+06
23	GB05-010260	Handbook of Glass.	1986	v.001, p.0244	2.692E+04

- Interpolated or extrapolated data at 700°C appear in red-purple color in the list.
- The glasses with no value are those which has only one value at another temperature, or which has no data in the range of $700 \pm 200^\circ\text{C}$ (default condition).
- When the user searches for 'Viscosity (100-1000C)', the calculation is done also for the other temperatures except 700°C.
- The interpolated or extrapolated values can be saved in the user's PC by clicking the [Save] icon. In case of the Internet edition, the save is unable.

4) Temperature-Property plot ([Temperature-Property Plot] window)



- Select a glass in the list, and by clicking the [Temperature-Property Plot] icon (the right [PLOT] icon), the [Temperature-Property Plot] window is shown.
- In the XY Plot, the interpolated or extrapolated plot-points appear in red-purple color. The style of plot-points and axis-scales can be changed on the pulldown menus under the graph.

(Ver. 7.2.1.0.05)

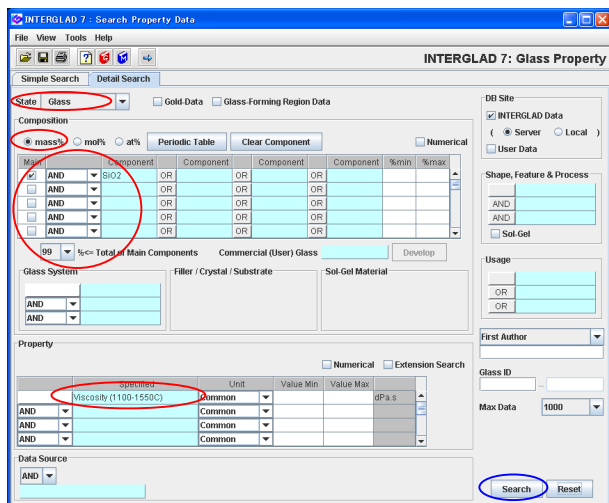
1.7 Analysis of high temperature properties – High temperature viscosity of silica glasses

Investigate temperature dependence ($>1100^{\circ}\text{C}$) on viscosity of silica glasses.

<Refer to B and C.3 of Chapter 3, and 2 and 3.3 of Chapter 4>

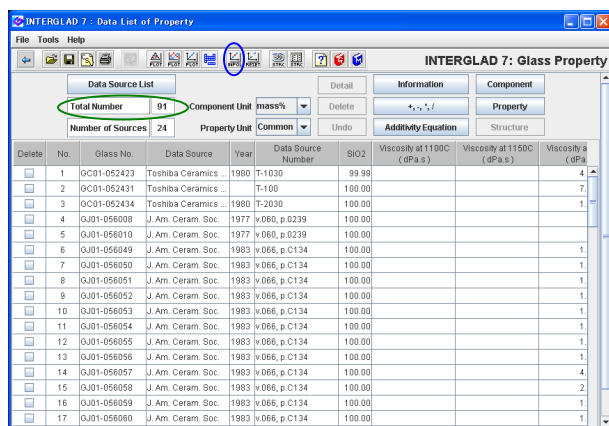
1) Specification of search conditions ([Search Property Data] window with [Detail Search] tag

→ Search

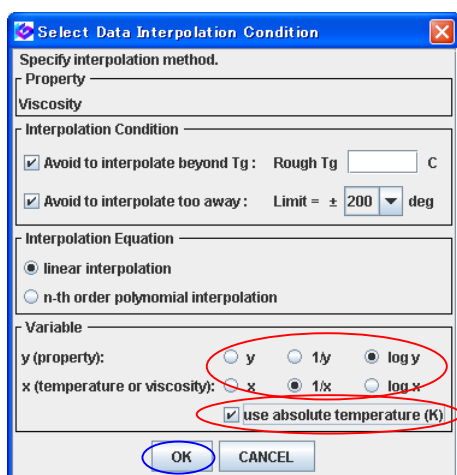


- In this example, glasses with $\text{SiO}_2 \geq 99$ mass% are searched as silica glasses.
- For viscosity, 'Viscosity (1100-1550C)' is selected.

2) Search result ([Data List of Property] window)



- 91 glasses are listed.



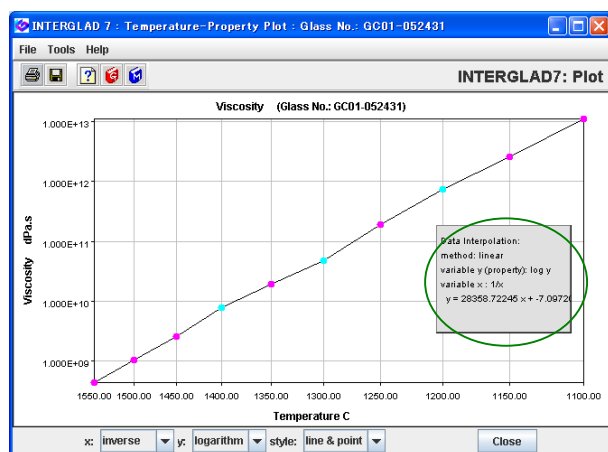
- Clicking the [Data Interpolation] icon opens the [Data Interpolation Condition] dialog box.
- In case of viscosity, the default of variable y is logy, and that of variable x (temperature) is 1/x. Check the [use absolute temperature (K)] checkbox.

[Data Interpolation Condition] dialog box

Delete	No.	Glass No.	Viscosity at 1100°C (dPa.s)	Viscosity at 1200°C (dPa.s)	Viscosity at 1250°C (dPa.s)	Viscosity at 1300°C (dPa.s)	Viscosity at 1350°C (dPa.s)	Viscosity at 1400°C (dPa.s)
	1	GC01-052423	1.230E+13	2.170E+13	4.000E+12	9.890E+11	2.700E+11	6.880E+10
	2	GC01-052431	1.094E+13	2.582E+12	7.400E+11	1.912E+11	4.800E+10	1.950E+10
	3	GC01-052434	6.193E+14	7.987E+13	1.300E+13	2.732E+12	6.900E+11	1.417E+11
	4	QJ01-056008						5.407E+11
	5	QJ01-056010						
	6	QJ01-056049			1.349E+09			
	7	QJ01-056050			1.776E+09			
	8	QJ01-056051			1.047E+09			
	9	QJ01-056052			1.905E+09			
	10	QJ01-056053			1.995E+09			
	11	QJ01-056054			1.259E+09			
	12	QJ01-056055			1.202E+09			
	13	QJ01-056056			1.000E+09			
	14	QJ01-056057			4.266E+08			
	15	QJ01-056058			2.630E+08			
	16	QJ01-056059			1.202E+09			
	17	QJ01-056060			1.122E+08			

- Interpolated or extrapolated values are shown in red-purple color in the list.

3) Temperature-property plot ([Temperature-Property Plot] window)



- Select a glass (No. 052431) with interpolated or extrapolated values, click the [Data Interpolation] icon, and the [Temperature-Property Plot] window opens. The registered (measured) values are in light-blue color, and the calculated values are in red-purple color.
- In this example, data of the specified temperature range 1100-1550°C are interpolated or extrapolated, as the temperature range for calculation is $\pm 200^\circ\text{C}$ (default condition) of the temperatures (1200, 1300, 1400°C) of the registered viscosity values. The interpolation or extrapolation equation is linear, $\log y = a(1/x) + b$ (where X: absolute temperature), which is shown in the figure.
- A Temperature-property plot shows data for each glass. When the user needs to compare data of glasses in a graph, save the data list by clicking the [CSV] icon, and make XY plots with data of specified glasses by using a spreadsheet software like Microsoft Excel.

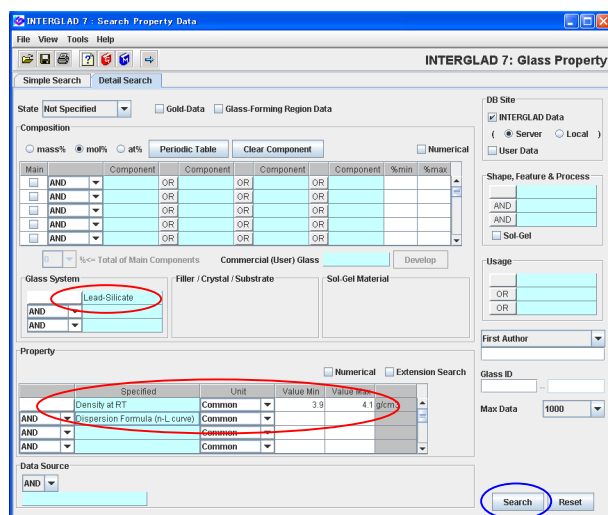
1.8 Figure of property equation – Refractive index dispersion of lead-silicate glasses

Investigate refractive index dispersion of lead-silicate glasses with 4 g/cm³ of density.

<Refer to B of Chapter 3, 2.3 of Chapter 4, and 3 of Chapter 6>

1) Specification of search conditions ([Search Property Data] window with [Detail Search] tag

→ Search



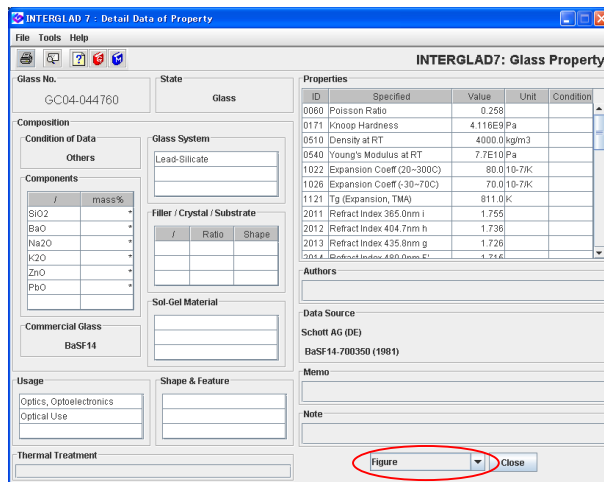
- Select 'Lead-Silicate' for the Glass System.
- Select 'Density at RT' and 'Dispersion Formula (n-L curve)' for the Property. Enter 3.9 and 4.1 in the cells of the Value Min and Value Max for 'Density at RT' respectively.

2) Search result ([Data List of Property] window)

Delete	No.	Glass No.	Data Source	Year	Data Source Number	Density at RT (g/cm³)	Const of Disp F A0	Const of Disp F A1
☐	5	OC04-044895	Schott AG (DE)	1981	BaSF52-702410	3.96	2.025	-1.306E-02
☐	15	OC04-048306	Ohara Inc (J)	1987	BaF01-683447	3.96	2.775	-1.480E-02
☐	16	OC04-048307	Ohara Inc (J)	1987	BaF03-686440	3.96	2.777	-1.141E-02
☐	17	OC04-048329	Ohara Inc (J)	1987	BaSF2-664359	3.96	2.693	-9.014E-03
☐	10	OC04-044759	Schott AG (DE)	1981	BaSF13-699386	3.97	2.806	-1.059E-02
☐	23	OC04-048338	Ohara Inc (J)	1987	BaSF01-702401	3.97	2.822	-9.918E-03
☐	33	OC04-071568	Corning Inc (US)	1985	FDC-C67-33	3.98	2.693	-8.394E-03
☐	11	OC04-044760	Schott AG (DE)	1981	BaSF14-700350	4.0	2.804	-1.012E-02
☐	14	OC04-048305	Ohara Inc (J)	1987	BaF13-669450	4.0	2.723	-9.936E-03
☐	30	OC04-066184	Hoya Corp (J)		FD19-667-331	4.01	2.697	-1.023E-02
☐	4	OC04-044692	Schott AG (DE)	1981	SF19-667330	4.02	2.694	-8.428E-03
☐	19	OC04-048334	Ohara Inc (J)	1987	BaSF7-702412	4.02	2.923	-1.090E-02
☐	22	OC04-049337	Ohara Inc (J)	1987	BaSF12-670293	4.02	2.716	-9.673E-03
☐	27	OC04-049357	Ohara Inc (J)	1987	SF19-667331	4.02	2.696	-1.026E-02
☐	28	OC04-066157	Hoya Corp (J)		BaFD2-664-359	4.02	2.692	-7.716E-03
☐	34	OC04-071569	Corning Inc (US)	1985	FB-C67-48	4.03	2.717	-7.780E-03
☐	39	OC04-074774	Pilkington (UK)		EDF-699301	4.04	2.788	-9.375E-03
☐	3	OC04-044688	Schott AG (DE)	1981	SF15-699301	4.06	2.79	-1.026E-02
☐	35	OC04-071571	Corning Inc (US)	1985	FeD-C72-32	4.06	2.708	-7.977E-03
☐	1	OC04-044678	Schott AG (DE)	1981	SF5-673322	4.07	2.711	-9.121E-03

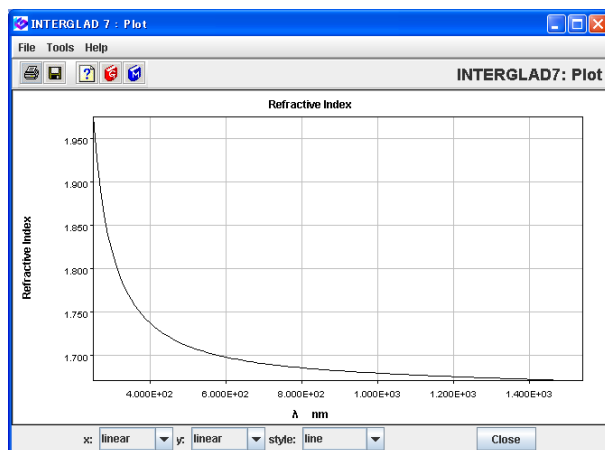
- 39 glasses are listed with the coefficient values of the equation.
- If the user sorts the values of the density, he/she finds 2 glasses with 4.0 g/cm³.
- Sellmeier Formula is also registered as another dispersion formula. When the search using Sellmeier Formula is performed in this case, no glass is found.
- In this example, a one-time search is not available under the condition of connecting the 2 formulas by OR.

3) Display of refractive index dispersion figure



[Detail Data of Property] window

- Open the [Detail Data of Property] window of a glass with 4.0 g/cm³ of density (No. 44760). Click 'CONST. DISP FORMULA' in the [Figure] pulldown menu on the bottom of the window, and a graph of the wavelength dispersion of refractive index appears.



[Plot/ Refractive Index] window

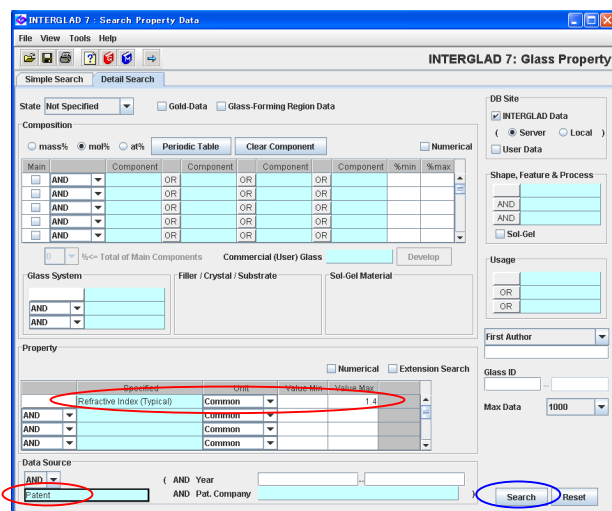
- The user can know the tendency of the refractive index change on wavelength by checking the curves of the other glasses in the same manner.
- In this example all the searched data are of catalogues and with no composition data. If the user searches by selecting only 'Density at RT' with 3.9-4.1 g/cm³ of 'Lead-Silicate' glasses in 'NOT Catalogue', he/she can assume the composition of the glass.

1.9 Patent search – Low refractive index glasses

Investigate compositions of low refractive index (1.4 or less) glasses on patents

<Refer to B and C.5 of Chapter 3, and 2 and 3.4 of Chapter 4>

- 1) Specification of search conditions ([Search Property Data] window with [Detail Search] tag)
→ Search



- Select “Refractive Index (Typical)” for the Property to collect many refractive index data. Enter ‘1.4’ for the Value Max of the Refractive Index.
- Select ‘Patent’ for the Data Source.

- 2) Search result ([Data List of Property] window)

No.	Glass No.	Data Source	Year	Data Source Number	Refractive index (Ty.)
1	GP25-048746	Japanese Patent	1979	A139917	1.356
2	GP25-048747	Japanese Patent	1979	A139917	1.394
3	GP25-048748	Japanese Patent	1979	A139917	1.355
4	GP25-048749	Japanese Patent	1979	A139917	1.343
5	GP25-056965	US Patent Owens	1979	A4142986	1.356
6	GP25-056966	US Patent Owens	1979	A4142986	1.394
7	GP25-056967	US Patent Owens	1979	A4142986	1.355
8	GP25-056968	US Patent Owens	1979	A4142986	1.343
9	TP01-061054	US Patent Battelle	1987	A4704299	1.4
10	GP60-070409	Japanese Patent	1983	A135152	1.383
11	GP60-070410	Japanese Patent	1983	A135152	1.377
12	GP60-070412	Japanese Patent	1983	A135152	1.384
13	GP60-095243	European Patent	1987	A0234455	1.337
14	GP60-095244	European Patent	1987	A0234455	1.332
15	GP60-190181	European Patent	1999	A0912453	1.4
16	GP60-190182	European Patent	1999	A0912453	1.4
17	GP60-190183	European Patent	1999	A0912453	1.39

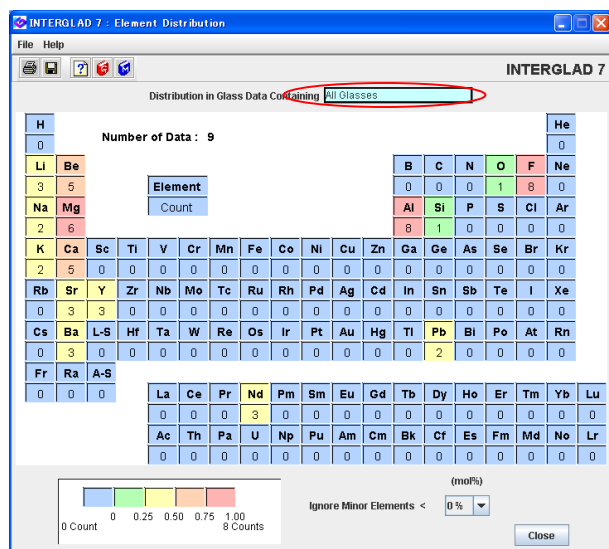
- 17 glasses are listed.

- 3) Utilization of the searched data

No.	Glass No.	Data Source	Year	Data Source Number	Glass System 1	Glass System 2	SiO ₂	Na ₂ O	P ₂ O ₅	LiF	NaF
1	GP25-048746	Japanese Patent	1979	A139917	Fluoro-Phosphate			*	*		24.4
2	GP25-048747	Japanese Patent	1979	A139917	Fluoro-Phosphate			*	*		15.0
3	GP25-048748	Japanese Patent	1979	A139917	Fluoro-Phosphate			*	*		25.0
4	GP25-048749	Japanese Patent	1979	A139917	Fluoro-Phosphate			*	*		16.2
5	GP25-056965	US Patent Owens	1979	A4142986	Phosphate	Fluoride		*	*		24.4
6	GP25-056966	US Patent Owens	1979	A4142986	Phosphate	Fluoride		*	*		15.0
7	GP25-056967	US Patent Owens	1979	A4142986	Phosphate	Fluoride		*	*		25.0
8	GP25-056968	US Patent Owens	1979	A4142986	Phosphate	Fluoride		*	*		16.2
9	TP01-061054	US Patent Battelle	1987	A4704299	Silica		100.00				
10	GP60-070409	Japanese Patent	1983	A135152	Fluoride						
11	GP60-070410	Japanese Patent	1983	A135152	Fluoride						
12	GP60-070412	Japanese Patent	1983	A135152	Fluoride						
13	GP60-095243	European Patent	1987	A0234455	Fluoride						
14	GP60-095244	European Patent	1987	A0234455	Fluoride						
15	GP60-190181	European Patent	1999	A0912453	Fluoride					9.00	
16	GP60-190182	European Patent	1999	A0912453	Fluoride					8.00	8.0
17	GP60-190183	European Patent	1999	A0912453	Fluoride					12.00	12.0

- In the [Data List of Property] window, by selecting ‘Glass System’ from the [Information] button, glass systems of the glasses are shown. And by clicking the [Select All] button from the [Component] button, all the components of the listed glasses appear.

4) Element analysis



- Elements of components of the searched glasses can be analyzed.
- By clicking the [Element Distribution] icon in the [Data List of Property] window, the [Element Distribution] window opens. By selecting 'All Glasses' of element in the [Distribution in Glass Data Containing] column, element distribution of all the listed glasses can be overviewed.
- In this example fluorides are main, and most of the glasses contain Al.
- As the Glass System, approximately half of the listed glasses are Phosphate or Fluoro-Phosphate, but the number of P is 0 in the Periodic Table of the [Element Distribution] window. Because in these cases P is registered as NaPO_3 , a complex oxide, and in such a case the calculated value of P_2O_5 is not registered, and only * for P_2O_5 appears. Compositions including * do not appear in the [Element Distribution] window.

5) Search glasses with low refractive index except patents (for reference)

INTERGLAD 7: Glass Property

Data Source List

Total Number: 54

Number of Sources: 23

Component Unit: mol%

Property Unit: Common

Delete	No.	Glass No.	Data Source	Year	Data Source Number	Refractive Index	Glass System 1	Glass System 2
	32	GJ00-145421	Phys. & Chem. Gla.	1991	v.032, p.0231	1.34	Fluoride	
	33	GJ01-148561	J. Non-Crystalline S.	1991	v.128, p.0069	1.34	Silica	
	34	GJ00-152063	J. Non-Crystalline S.	1993	v.161, p.0210	1.2	Fluoride	
	35	GJ10-157836	J. Non-Crystalline S.	1994	v.167, p.0180	1.339	Borate	Other Oxide
	36	GJ10-157837	J. Non-Crystalline S.	1994	v.167, p.0180	1.25	Borate	Other Oxide
	37	GJ02-165498	Glastech. Ber.	1996	v.069, p.0216	1.387	Alkali Silicate	Other Oxide
	38	GJ02-165499	Glastech. Ber.	1996	v.069, p.0216	1.387	Alkali Silicate	Other Oxide
	39	GJ02-165500	Glastech. Ber.	1996	v.069, p.0216	1.369	Alkali Silicate	Other Oxide
	40	GJ03-172323	J. Non-Crystalline S.	1997	v.212, p.0055	1.14	Alkaline-earth Silicate	Alumino-Silicate
	41	GJ03-172324	J. Non-Crystalline S.	1997	v.212, p.0055	1.22	Alkaline-earth Silicate	Alumino-Silicate
	42	GJ03-172325	J. Non-Crystalline S.	1997	v.212, p.0055	1.38	Alkaline-earth Silicate	Alumino-Silicate
	43	GJ00-174911	Data Book of Glass.	1991	v.001, p.0179	1.27	Fluoride	
	44	GJ10-207463	Glastech. Ber.	2001	v.074, p.0038	1.35	Borate	
	45	GJ00-225306	Materials Science F.	1985	v.005, p.0145	1.4	Fluoride	
	46	GJ10-239888	Bull. Mater. Sci.	1999	v.022, p.1055	1.25	Borate	Halide (Except Fluoride)
	47	GJ27-239945	Bull. Mater. Sci.	2003	v.026, p.0639	1.3	Lead	Other Oxide
	48	GJ27-239947	Bull. Mater. Sci.	2003	v.026, p.0639	1.39	Lead	Other Oxide
	49	MJ02-266029	Glass Phys. & Chem.	2005	v.031, p.0602	1.4	Alkali Silicate	
	50	MJ02-266030	Glass Phys. & Chem.	2005	v.031, p.0602	1.3	Alkali Silicate	
	51	MJ02-266031	Glass Phys. & Chem.	2005	v.031, p.0602	1.3	Alkali Silicate	
	52	GJ28-292329	J. Material Science	2009	v.044, p.5800	1.309	Tellurite	Other Oxide
	53	GJ28-292330	J. Material Science	2009	v.044, p.5800	1.25	Tellurite	Other Oxide

- When the search is performed under condition of 'Not Patent' for the Data Source, 54 glasses are listed.
- The Glass Systems of these glasses are Fluoride, Alkali-Silicate, Alkaline-earth Silicate, Tellurite, etc. Patents of these glasses are not registered in INTERGLAD.

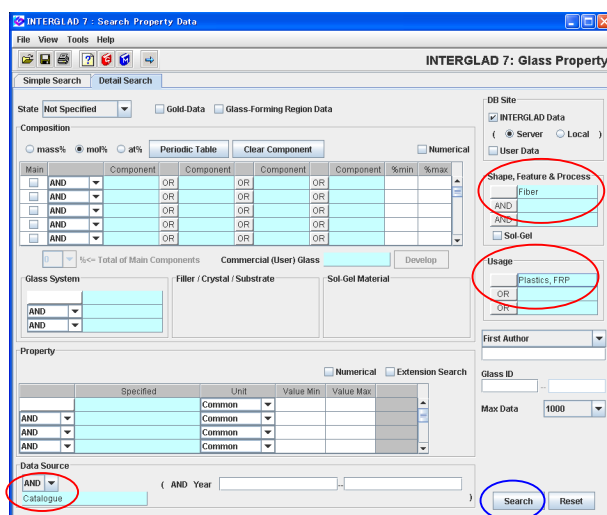
1.10 Search of commercial glasses – High strength glass fiber for FRP

Investigate commercial glasses of high strength glass fiber for FRP.

<Refer to B of Chapter 3, and 2 of Chapter 4>

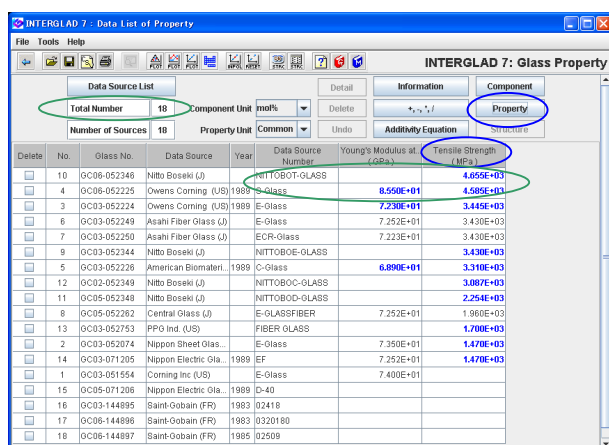
1) Specification of search conditions ([Search Property Data] window with [Detail Search] tag)

→ Search

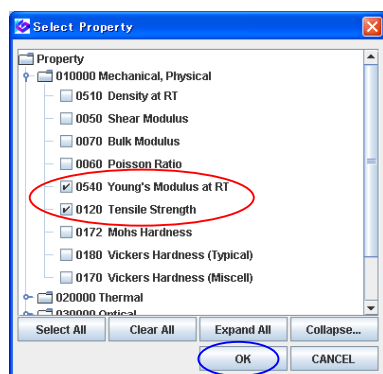


- Select 'Fiber' after opening 'Appearance/Shape/Linear' in the [Shape, Feature & Process] column.
- Select 'Plastics, FRP' in 'Material' by clicking the [Usage] column.
- Select 'Catalogue' for the [Data Source] column.

2) Search result ([Data List of Property] window)



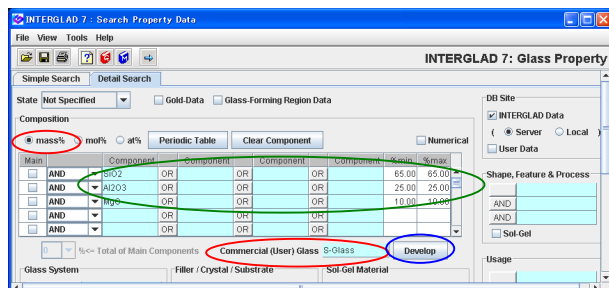
- 18 glasses are listed. These are found to be data of 10 manufacturers in the 'Data Source' column.
- Open the [Select Property] dialog box by clicking the [Property] button.
- Check in the 'Tensile Strength' and 'Young's Modulus at RT' checkboxes, and both the data are shown. Tensile strength and Young's modulus are important properties for high strength glass fiber.



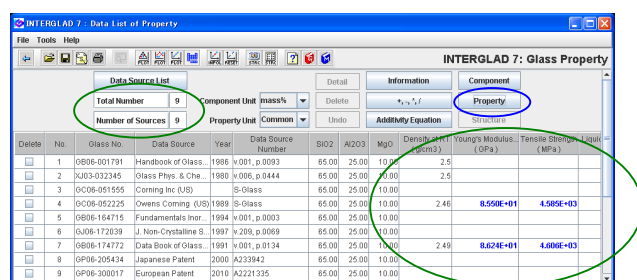
- By sorting the 'Tensile Strength' column, glasses with high strength can be found. (NITTOBO T-Glass and S-Glass are the highest.)

[Select Property] dialog box

3) Investigation of a searched glass

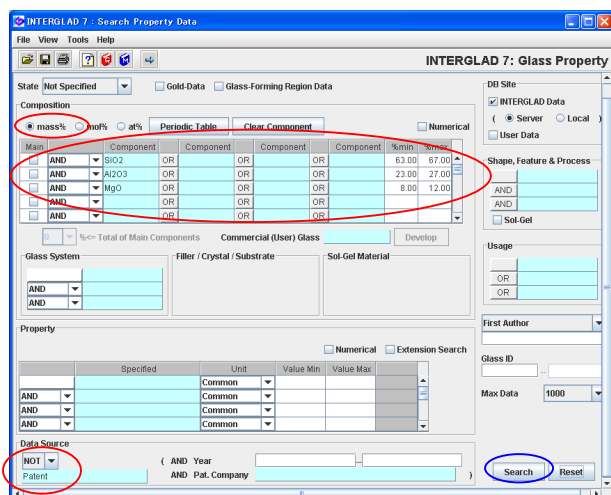


- Here S-glass with high tensile strength and high Young's modulus is investigated.
- Go back to the [Search Property Data] window, select 'S-Glass' in the [Commercial (User) Glass] column, and click the [Develop] button. Then search with no specification of the Data Source.
- In this case values of %min and %max are the same, because the glass compositions registered have no difference.

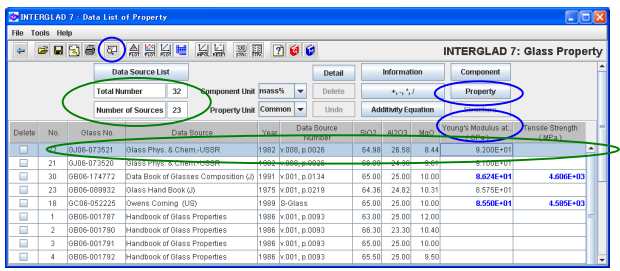


- 9 glasses (9 data sources) are listed. When the search is performed without clicking the [Develop] button, only 3 glasses are listed. By developing the composition, it is found that data of Journals, etc. besides catalogues are also searched.
- By clicking 'Select All' button in the [Select Property] dialog box from the [Property] button, all the property data registered are shown in the list.

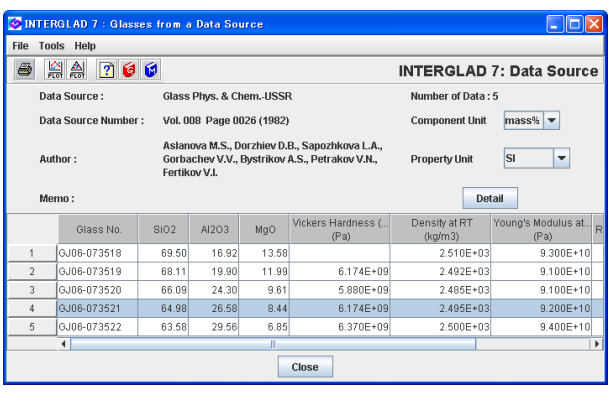
4) Investigation of data around S-Glass



- Information of glasses around S-Glass is collected.
- $\pm 2\%$ values of %min and %max are set as a search condition.
- Select 'NOT Patent' for the Data Source.



- 32 glasses of 23 data sources are listed. When patents are also included in the search condition, 87 glasses of 43 data sources are listed.
- List the values of ‘Tensile Strength’ and ‘Young’s Modulus at RT’ from the [Property] button, and sort the values of Young’s Modulus. By this procedure the mechanical property of the glasses around the S-Glass composition are shown.



- Clicking the [Glasses from a Data Source] icon after selecting the glass GJ06-073521 with the highest Young’s modulus opens the [Glasses from a Data Source] window of the glass. All the data in this data source can be checked.

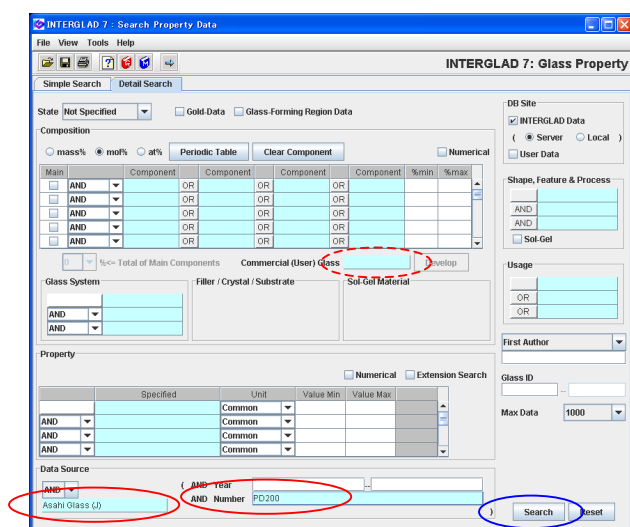
[Glasses from a Data Source] window

1.11 Estimate of a commercial glass composition

Composition values are usually not given in commercial glasses. However the compositions may be estimated from patent data. Here, the composition of PD200 of Asahi Glass is estimated.

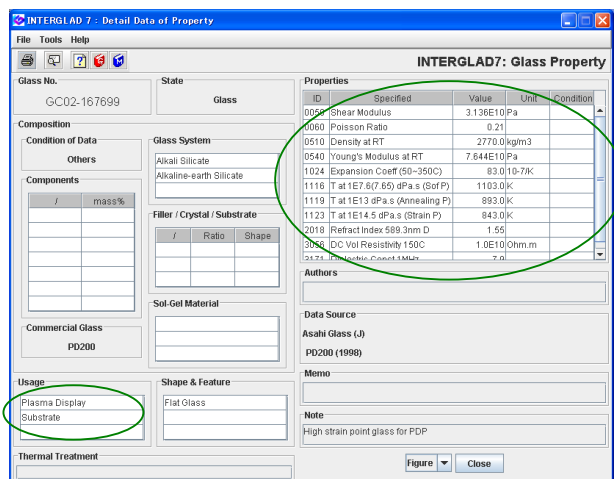
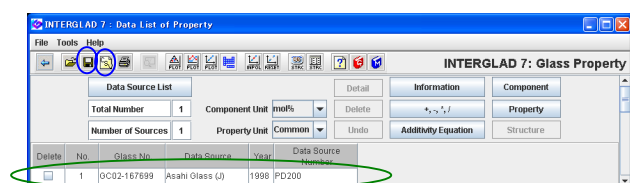
< Refer to B of Chapter 3, and 2 of Chapter 4 >

- 1) Specification of search conditions ([Search Property Data] window with [Detail Search] tag)
→ Search



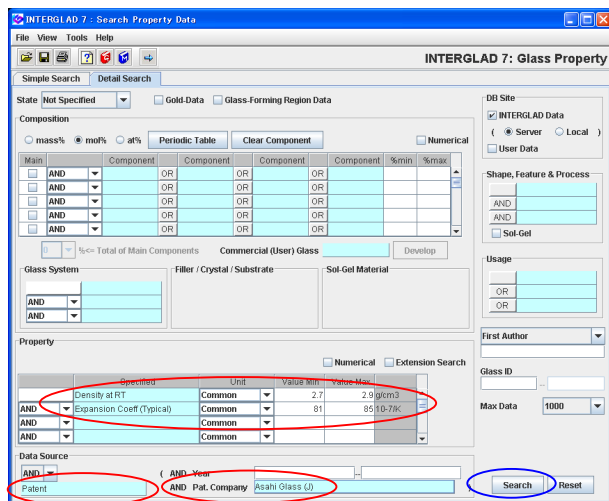
- Select 'Asahi Glass (J)' in 'Catalogue' of the Data Source, and select 'PD200' in the [AND Number] column, which appears on the right side of the [Data Source] column.
- Instead of the above search condition, selection of 'P/PD200' in the [Commercial (User) Glass] column brings the same result.

- 2) Search result ([Data List of Property] window → [Detail Data of Property] window)

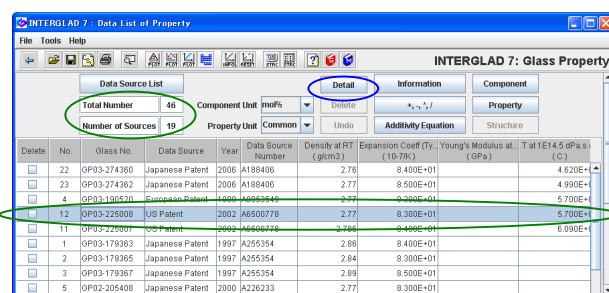


- The glass data of PD200 appears.
- Check the properties and usages of the glass in the [Detail Data of Property] window, and print the window.
- The above procedure can be replaced with the following. Exhibit all the property data in the list by selecting 'Select All' in the [Select Property] dialog box from the [Property] button. And save the data of the table from the [CSV] icon or save the window using the [Save] icon.

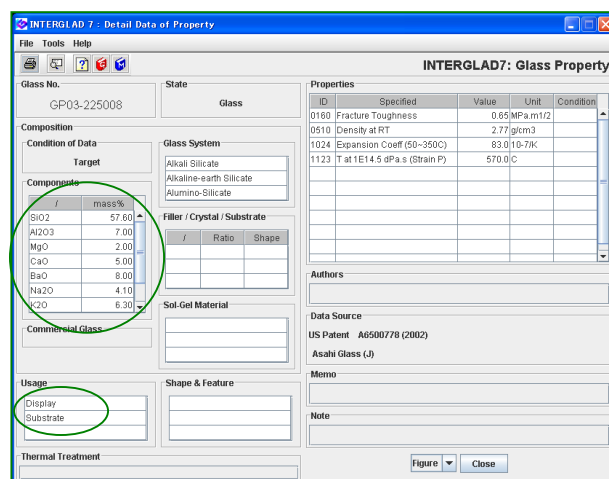
3) Search for composition estimate ([Search Property Data] window → [Data List of Property] window → [Detail Data of Property] window)



- Go back to the [Search Property Data] window, and click the [Reset] button.
- Select 'Density at RT' and 'Thermal Coeff (Typical)' for the [Property] column as typical items of the searched properties of PD200.
- Set value ranges (min% and max%) of the properties of PD200 as follows.
Density: 2.7-2.9 g/cm³
Thermal Coeff: 81-85 × 10⁻⁷/K
- Select 'Patent' for the [Data Source] column, and 'Asahi Glass (J)' for the [AND Pat. Company] column.



- 44 glasses are listed, and 4 of the glasses have the same values of Density and Thermal Coeff as those of PD200.
- To select a fit composition, add data of 'Young's Modulus at RT' and 'T at 1E14.5 dPa.s (Strain P)' to the list using the [Property] button.



- 2 glasses with the same Strain P as that of PD200 are found (190520, 225008). Note the difference of C and K temperature units. The composition of the 2 glasses is almost the same. 'Display' and 'Substrate' are registered as Usage in the [Detail Data of Property] window of 225008. This usage is fit to that of PD200. In this way the user can estimate the composition of the commercial glass PD200.

1.12 Search from usage (application) – Seal glasses for semiconductor package

Investigate seal glasses for semiconductor package.

<Refer to B, C.2 and C.5 of Chapter 3, and 2, 3.2 and 3.4 of Chapter 4>

1) Specification of search conditions ([Search Property Data] window with [Detail Search] tag)

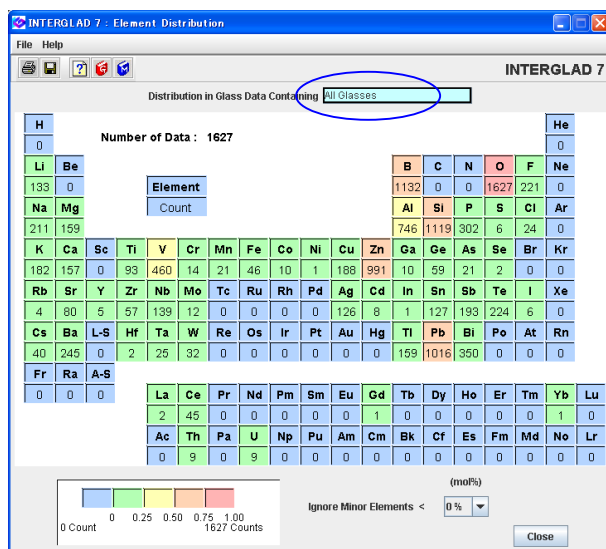
→ Search→ Search result ([Data List of Property] window)

- Select 'Electronics, Electrical/ Solder Glass, Sealing Glass/ for Semiconductor Package' for the Usage.

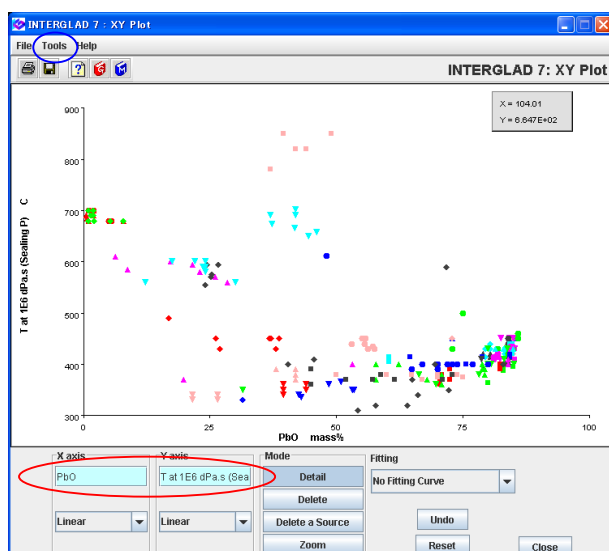
No.	Glass No.	Data Source	Year	Data Source Number	State	Shape 1	Shape 2	Shape 3	Shape 4
725	OC99-099005	Ishizuka Glass (J)		IG-9380	Glass	Low Melting	Disk	Fiber	Powder, Frit
726	OC99-099006	Ishizuka Glass (J)		IG-9381	Glass	Low Melting	Disk	Powder, Frit	Fiber
727	OC99-099007	Ishizuka Glass (J)		IG-9370	Glass	Low Melting	Disk	Powder, Frit	Fiber
728	OC99-099008	Ishizuka Glass (J)		IG-9330	Glass	Low Melting	Disk	Fiber	Powder, Frit
729	OC99-099009	Ishizuka Glass (J)		IG-9350	Glass	Low Melting	Disk	Fiber	Powder, Frit
730	OC99-099010	Ishizuka Glass (J)		IG-0580	Glass	Low Melting	Disk	Powder, Frit	Fiber
731	OC99-099011	Ishizuka Glass (J)		IG-0581	Glass	Low Melting	Disk	Fiber	Powder, Frit
732	OC99-099012	Ishizuka Glass (J)		IG-1320	Glass	Low Melting	Disk	Powder, Frit	Fiber
733	OC99-099013	Ishizuka Glass (J)		IG-1330	Glass	Low Melting	Disk	Fiber	Powder, Frit
734	OC99-099014	Ishizuka Glass (J)		IG-1560	Glass	Low Melting	Disk	Powder, Frit	Fiber
735	OC99-099015	Ishizuka Glass (J)		IG-1561	Glass	Low Melting	Disk	Fiber	Powder, Frit
736	OC99-099016	Ishizuka Glass (J)		IG-1590	Glass	Low Melting	Powder, Frit	Disk	Fiber
737	OC99-099017	Ishizuka Glass (J)		IG-2540	Glass	Low Melting	Disk	Fiber	Powder, Frit
738	OC99-099018	Ishizuka Glass (J)		IG-2541	Glass	Low Melting	Powder, Frit	Disk	Fiber
739	OC99-099019	Ishizuka Glass (J)		IG-3460	Glass	Low Melting	Disk	Fiber	Powder, Frit
740	CP03-100567	Japanese Patent	1989	A014127	Composite	Thick Film	Glass Cer.	Enamel, GL	

- 1703 glasses are listed. From the Data Source, it is found that most of the glasses are of Patent, 59 glasses are of Catalogue, and 35 glasses are of Journal. In case of Catalogue, the user can have information of commercial name (No., etc). from the Data Source Number.
- By adding 'State' to the list from the [Information] button, the user knows that 'Glass-Ceramics,' 'Composite' and 'Modified Glass' are included besides 'Glass.'
- By adding 'Shape, Feature & Manufacturing Process' from the [Information] button, various information is shown, 'Powder,' 'Frit' for the Shape, 'Non Lead,' 'Non-Alkali' for the Composition, 'Low Melting' for the Property.

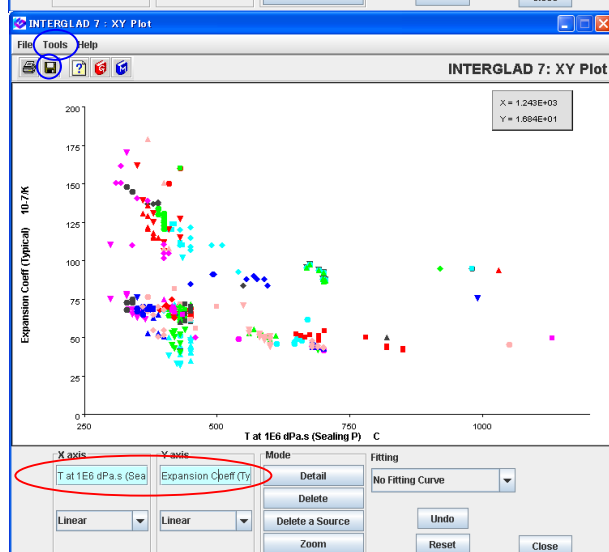
2) Analysis ([Element Distribution] window, [XY Plot] window)



- To obtain information about component, open the [Element Distribution] window by clicking the [Element Distribution] icon, and select 'All Glasses' in the [Distribution in Glass Data Containing] column.
- Compositions containing B, Si, Zn, Al, or V (except O) are comparatively many.
- Return to the [Data List of Property] window, and add data of 'T at 1E6 dPa.s (Sealing P)' from the [Property] button. The Sealing Point varies greatly from 280 to 1130°C.

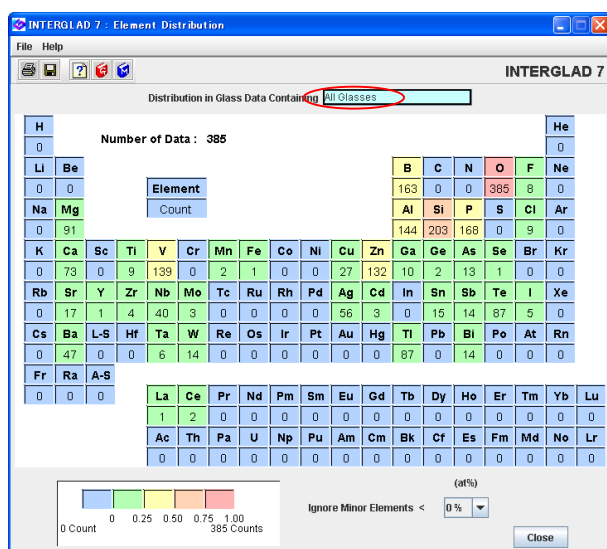
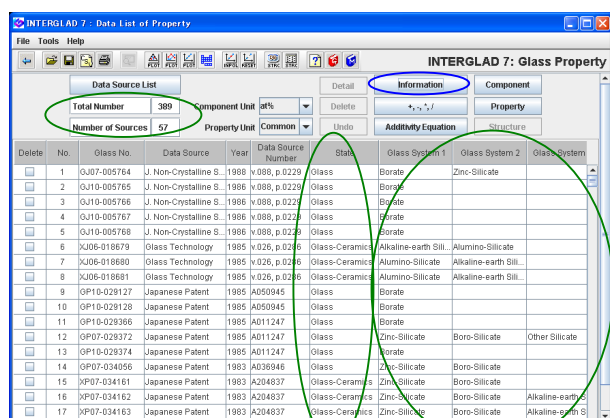
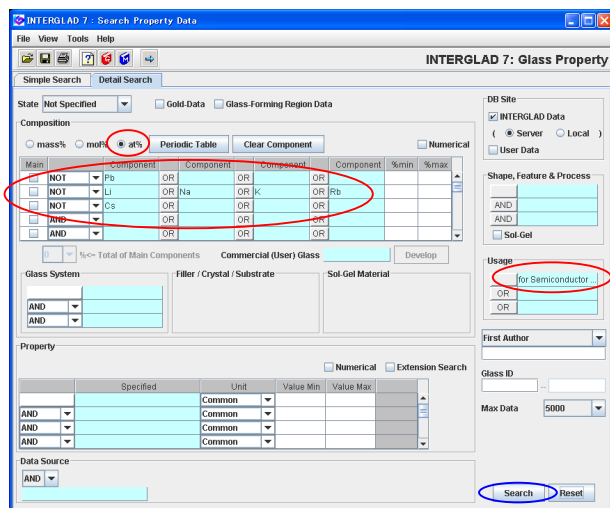


- Open the [XY Plot] window from the [XY Plot] icon. Select 'PbO' for the X axis and 'T at 1E6 dPa.s (Sealing P)' for the Y axis. The plot-points of the Sealing P are distributed in a wide range of temperature. When the PbO content is high, the Sealing P is concentrated in a range of low temperatures.

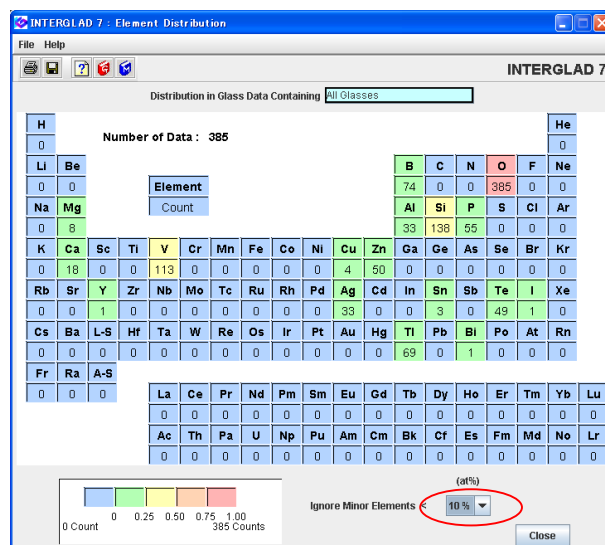


- Draw a XY Plot of Sealing P vs. Expansion Coeff. The thermal expansion coefficient varies widely in the low Sealing P. range. So, in such a Sealing P. range, the user can select a sealing glass according to the purpose of application.
- Value range and style of axes can be changed by using 'Tools/ Option' as shown in these figures. Ex. Style of Sealing P: 5.0E+02 → 500.
- The [XY Plot] window can be saved as a JPEG file in the user's PC by clicking the [Save] icon.

3) Investigation of sealing glasses with non-lead and non-alkali ([Search Property Data] window, [Data List of Property] window, [Element Distribution] window)



- Select 'at%' for the component unit. Select Pb, Li, Na, K, Rb, Cs in the [Periodic Table] dialog box, and select 'NOT' in each [AND, OR, NOT] pulldown menu. Selection of alkali elements like the example window is also available.
- 389 glasses are listed. Search with plural 'NOT' takes time especially in the case of CD Full Function edition.
- By adding 'State' and 'Glass System' to the list, it is found that 'Glass,' 'Composite' and 'Glass-Ceramics' for the State, and 'Borate,' 'Boro-Silicate,' 'Alumino-Silicate,' 'Phosphate,' 'Zinc-Silicate,' 'Tellulite,' etc. for the Glass System are listed.
- When the user opens the [Element Distribution] window, he/she finds that many glasses contain Si, P, B, Al, V or Zn except O. The contents of Pb and alkali elements are both 0 at%.
- By selecting '10%' in the [Ignore Minor Elements] pulldown menu, only the main elements with ≥ 10 at% are indicated.



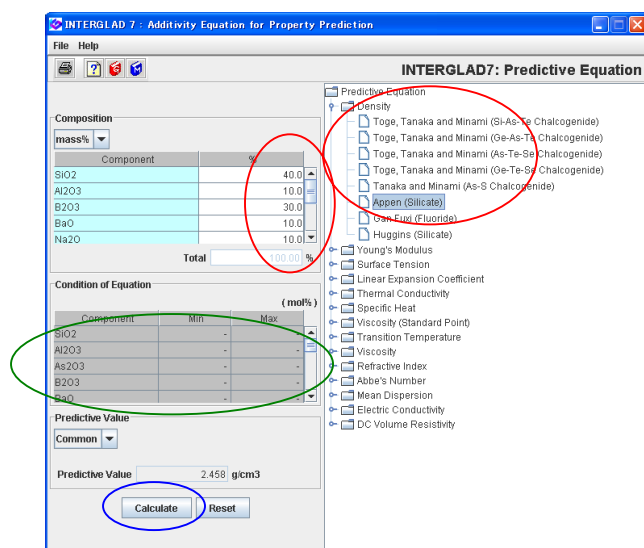
2. Property Prediction by Additivity Equations

2.1 Property prediction of glasses with a specified composition – Boro-silicate glasses

Predict density, thermal expansion coefficient and refractive index of boro-silicate glasses with SiO₂ 40%, B₂O₃ 30%, Al₂O₃ 10%, Na₂O 10% and BaO 10% (mass%).

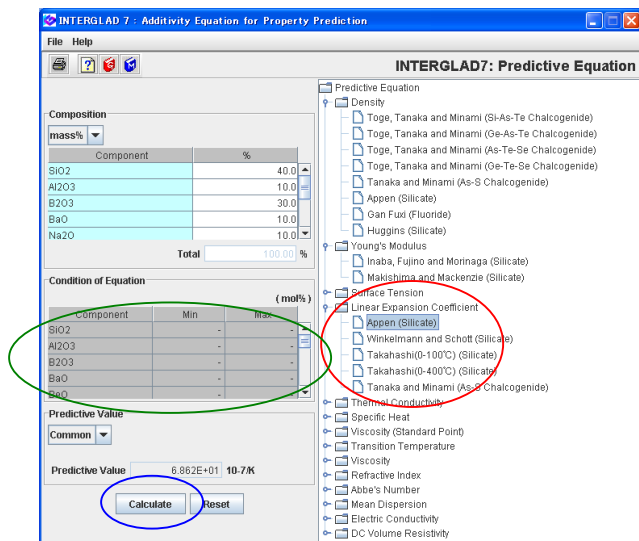
<Refer to D.1 of Chapter 3, 4.1 of Chapter 4, and 1 of Chapter 6>

1) Prediction of density ([Additivity Equation for Property Prediction] window)



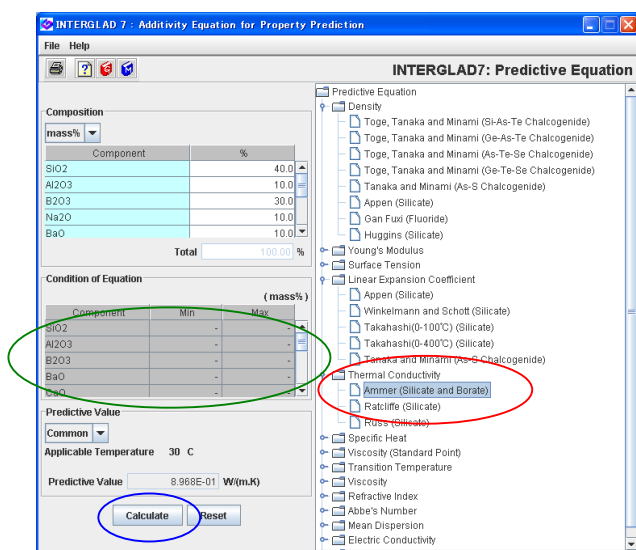
- Open the [Additivity Equation for Property Prediction] window, and select 'Appen(Silicate)' after developing 'Density' in the [Predictive Equation] menu on the right-hand part of the window.
- The [Condition of Equation] appears on the left-hand part. Check if the values of the components of glasses to be predicted are included in the condition.
- Select components required for the property prediction, and enter each value in the [Composition %] column. Plural components can be selected in one time by using the Ctrl key. In this example the component unit is mass%.
- After clicking the [Calculate] button, the predictive value 2.458 g/cm³ appears in the [Predictive Value] column.

2) Prediction of thermal expansion coefficient



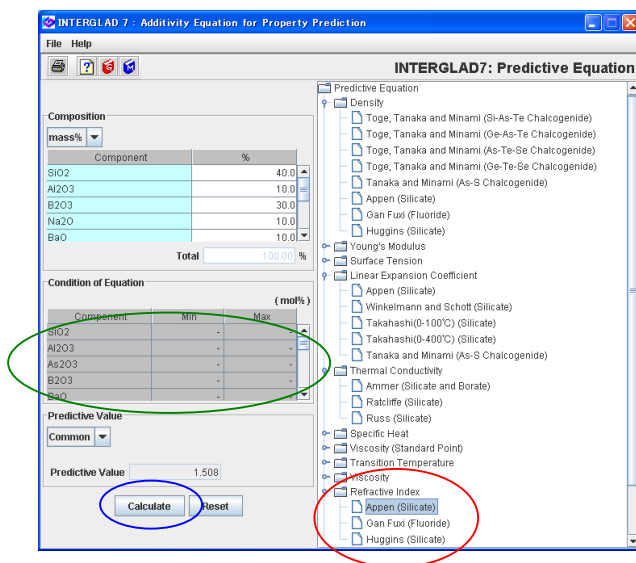
- In case of prediction of the other properties for the same composition, property prediction can be performed only by reselecting the property equation.
- Select 'Appen(Silicate)' after developing 'Linear Expansion Coefficient' in the [Predictive Equation] menu.
- Clicking the [Calculate] button shows the predictive value 6.862×10^{-6} /K in the [Predictive Value] column.

3) Prediction of thermal conductivity



- Select 'Ammer(Silicate and Borate)' after developing 'Thermal Conductivity' in the [Predictive Equation] menu.
- By clicking the [Calculate] button, the predictive value 8.968×10^{-1} W/(mK) (30°C) appears in the [Predictive Value] column.
- In this example, equations of 'Ratcliffe(Silicate)' and 'Russ(Silicate)' can also be used, and 8.349×10^{-1} W/(mK) (0°C) and 9.256×10^{-1} W/(mK) (0°C) are obtained respectively. The user can compare the results by the difference of additivity equations.

4) Prediction of refractive index



- Select 'Appen(Silicate)' after developing 'Refractive Index' in the [Predictive Equation] menu.
- By clicking the [Calculate] button, the predictive value 1.508 appears in the [Predictive Value] column.
- Predictive values of various properties can be calculated for a composition as described above, but in many cases calculations are not possible owing to various composition limitation of equations.

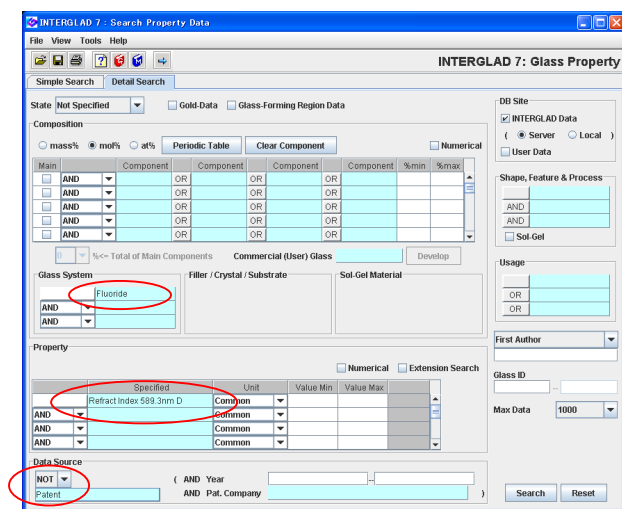
< Refer to 1 of Chapter 6 >

2.2 Comparison of calculated values by an additivity equation with fact data – Refractive index of fluoro-glasses

Compare refractive index values of fluoro-glasses calculated by Gan Fuxi equation with the fact data of the glasses.

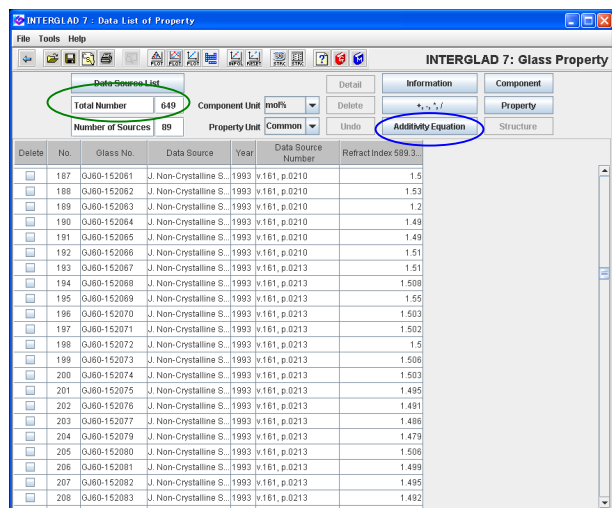
<Refer to B and D.1 of Chapter 3, 2 and 4.1 of Chapter 4, and 1 of Chapter 6>

- 1) Specification of search conditions ([Search Property Data] window with [Detail Search] tag)
→ Search

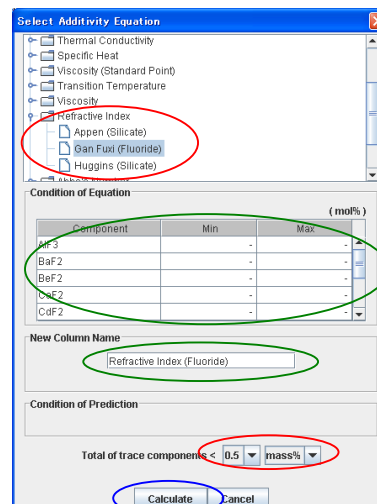


- Select 'Fluoride' for the Glass System, 'Refract Index 589.3nmD' for the Property, and set 'NOT Patent' for the Data Source.
- In this example, '589.3nm D-line' is selected as the Refractive Index, because Gan Fuxi equation is that to calculate refractive index of D-line.

- 2) Search result ([Data List of Property] window)



- 649 glasses are listed with the data of the refractive index.
- By clicking the [Additivity Equation] button, the [Select Additivity Equation] dialog box opens. Select 'Refractive Index/ Gan Fuxi(Fluoride)' and click the [Calculate] button. In this example '0.5' mass% is set as 'Total of trace compositions (impurities) <.'



[Select Additivity Equation] dialog box

INTERGLAD 7: Data List of Property

File Tools Help

INTERGLAD 7: Glass Property

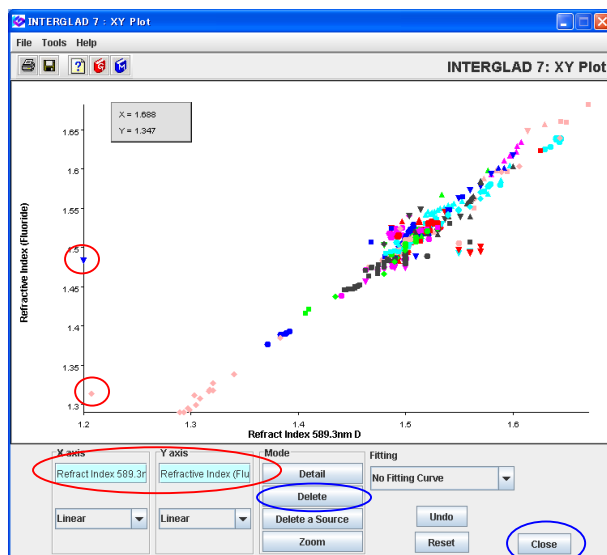
Data Source List

Total Number: 649
Component Unit: mol%
Property Unit: Common
Delete
Additivity Equation

No.	Glass No.	Data Source	Year	Data Source Number	Refractive Index (Fluoride)	Refractive Index 589.3
187	QJ80-152061	J. Non-Crystalline S.	1993	v161, p.0210	1.495	1.5
188	QJ80-152062	J. Non-Crystalline S.	1993	v161, p.0210	1.523	1.53
189	QJ80-152063	J. Non-Crystalline S.	1993	v161, p.0210	1.482	1.2
190	QJ80-152064	J. Non-Crystalline S.	1993	v161, p.0210	1.484	1.49
191	QJ80-152065	J. Non-Crystalline S.	1993	v161, p.0210	1.495	1.49
192	QJ80-152066	J. Non-Crystalline S.	1993	v161, p.0210	1.488	1.51
193	QJ80-152067	J. Non-Crystalline S.	1993	v161, p.0213	1.51	1.51
194	QJ80-152068	J. Non-Crystalline S.	1993	v161, p.0213	1.508	1.508
195	QJ80-152069	J. Non-Crystalline S.	1993	v161, p.0213	1.506	1.55
196	QJ80-152070	J. Non-Crystalline S.	1993	v161, p.0213	1.503	1.503
197	QJ80-152071	J. Non-Crystalline S.	1993	v161, p.0213	1.501	1.502
198	QJ80-152072	J. Non-Crystalline S.	1993	v161, p.0213	1.499	1.5
199	QJ80-152073	J. Non-Crystalline S.	1993	v161, p.0213	1.508	1.506
200	QJ80-152074	J. Non-Crystalline S.	1993	v161, p.0213	1.503	1.503
201	QJ80-152075	J. Non-Crystalline S.	1993	v161, p.0213	1.498	1.495
202	QJ80-152076	J. Non-Crystalline S.	1993	v161, p.0213	1.484	1.491
203	QJ80-152077	J. Non-Crystalline S.	1993	v161, p.0213	1.491	1.486
204	QJ80-152079	J. Non-Crystalline S.	1993	v161, p.0213	1.484	1.479
205	QJ80-152080	J. Non-Crystalline S.	1993	v161, p.0213	1.508	1.506
206	QJ80-152081	J. Non-Crystalline S.	1993	v161, p.0213	1.504	1.499
207	QJ80-152082	J. Non-Crystalline S.	1993	v161, p.0213	1.495	1.495
208	QJ80-152083	J. Non-Crystalline S.	1993	v161, p.0213	1.49	1.41

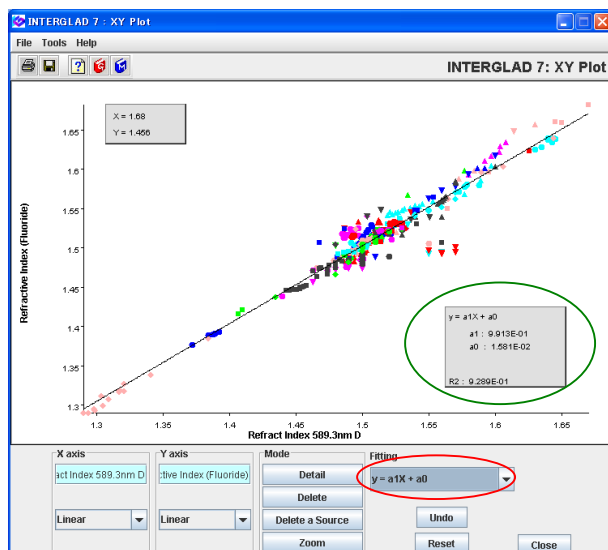
- The values calculated by the additivity equation appear in the [Data List of Property] window. The label 'Refractive Index (Fluoride)' is in pink-color.

3) XY Plot to compare predictive values with measured values ([XY Plot] window)



- Open the [XY Plot] window from the [XY Plot] icon, and select 'Refract Index 589.3nm D' for the X axis and 'Refractive Index (Fluoride)' for the Y axis. Relation between the measured values and the calculated values are shown.

- To delete 2 separated plot-points, click the 2 plot-points after clicking the [Delete] button.



- After clicking the [Close] button, reopen the [XY Plot] window. Select ' $y = a_1x + a_0$ ' in the [Fitting] column, and a fitting curve appears. The user can obtain a good fitting equation of the measured and calculated values in this example.

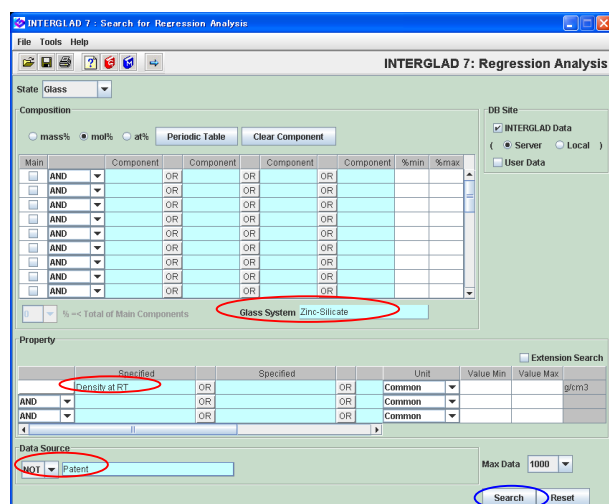
3. Property Prediction & Material Designing (Composition Optimization) by Multiple Regression Analysis

3.1 Obtaining an additivity equation of a property — Density of zinc-silicate glasses

Obtain a multiple regression equation of density at RT for zinc-silicate glasses.

<Refer to D.2 of Chapter 3, 4.2-4.5 of Chapter 4>

1) Specification of search conditions ([Search for Regression Analysis] window) → Search

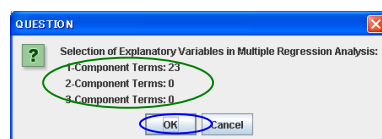
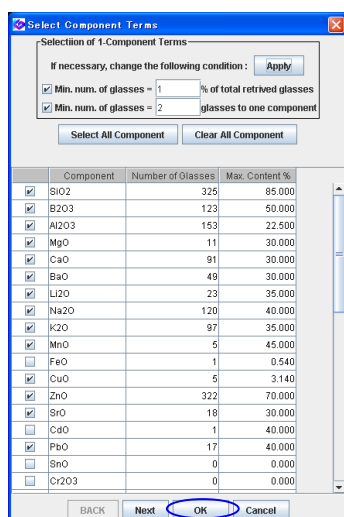


- Open the [Search for Regression Analysis] window.
- Select 'Glass' (default) for the State.
- Select 'Zinc-Silicate' for the Glass System, 'Density at RT' for the Property, and 'NOT Patent' for the Data Source.

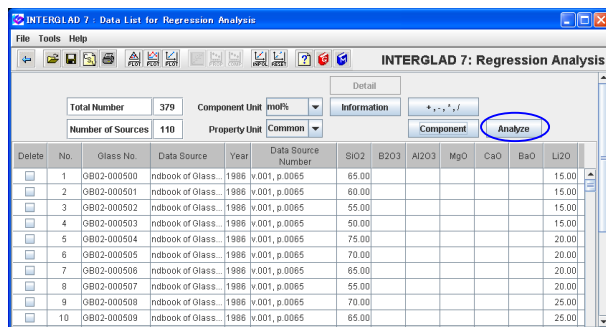
2) Search result ([Data List for Regression Analysis] window) → Selection of explanatory variables ([Selection of 1, 2, 3-Component Terms] dialog boxes)

No.	Glass No.	Data Source	Year	Density at RT (g/cm3)	Density at RT (Predictive Value)	Density at R (Residual)
1	GB02-000500	Handbook of Glass	1906	2.74		
2	GB02-000501	Handbook of Glass	1906	2.867		
3	GB02-000502	Handbook of Glass	1906	2.99		
4	GB02-000503	Handbook of Glass	1906	3.115		
5	GB02-000504	Handbook of Glass	1906	2.405		
6	GB02-000505	Handbook of Glass	1906	2.51		
7	GB02-000506	Handbook of Glass	1906	2.636		
8	GB02-000507	Handbook of Glass	1906	2.895		
9	GB02-000508	Handbook of Glass	1906	2.439		
10	GB02-000509	Handbook of Glass	1906	2.55		

- 379 glasses are listed.
- Open the [Selection of 1, 2, 3-Component Terms] dialog boxes by clicking the [Component] button, and specify component terms for a multiple regression equation.
- In this example, click the [OK] button in the [Select Component Terms] dialog box for the Selection of 1-component Terms at default setting.
- By this command the explanatory variables are limited to 1-component terms. Check the number of the component terms in the [Question] dialog box.

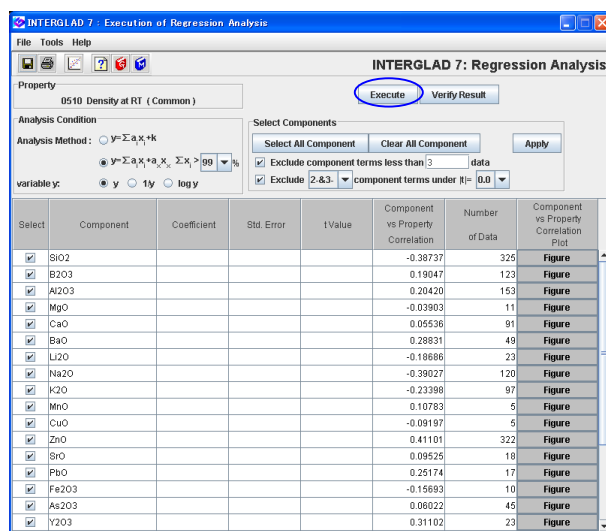


1-Component Terms: 23.

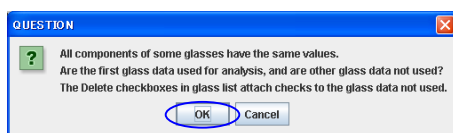


- By clicking the [Analyze] button, the [Execution of Regression Analysis] window opens.

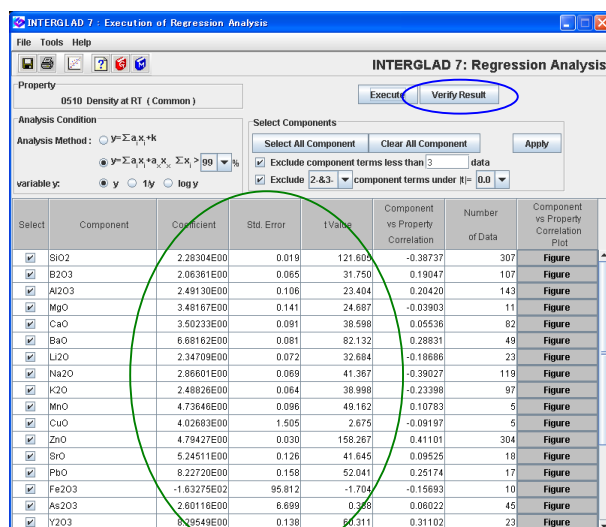
3) Execution of multiple regression analysis ([Execution of Regression Analysis] window)



- Execute the multiple regression analysis at default setting by clicking the [Execute] button.

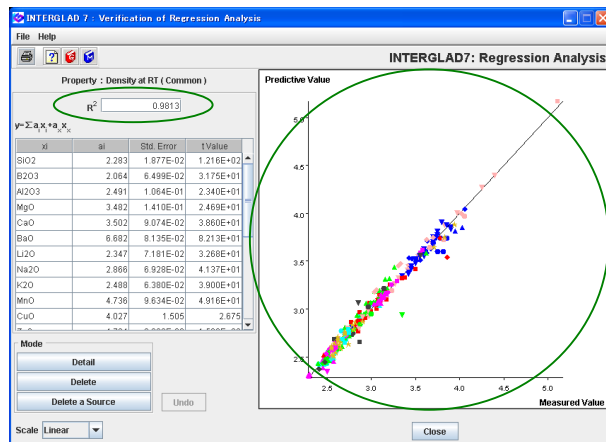


- A [Question] dialog box appears. Check the dialog, and click the [OK] button.



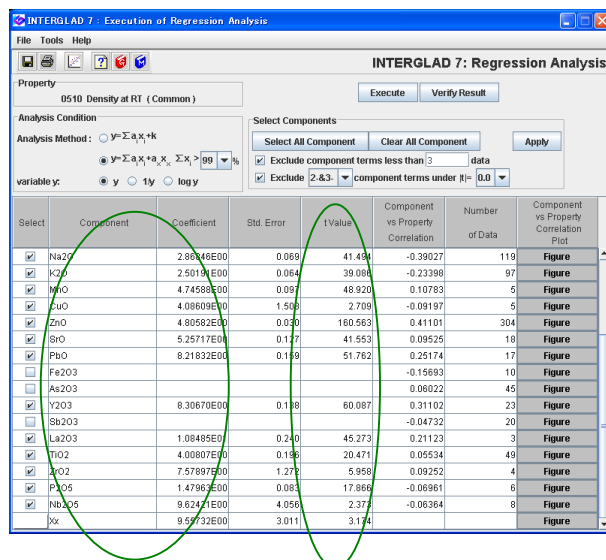
- The regression coefficients, the standard errors and t values appear in the table after the calculation.
- By clicking the [Verify Result] button, open the [Verification of Regression Analysis] window.

4) Verification of regression analysis ([Verification of regression analysis] window)

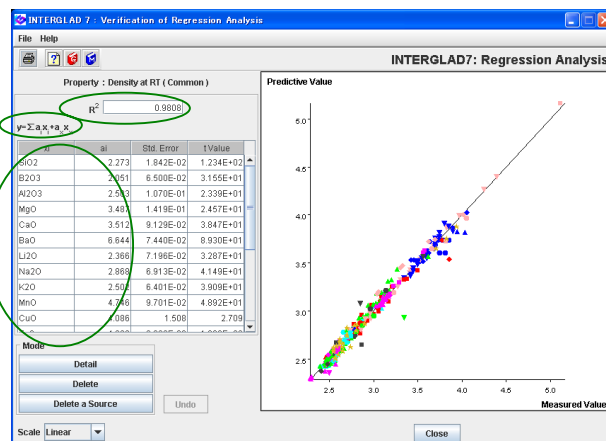


- In this example a high contribution rate R^2 (0.98) is obtained. The scattering of the plot-points is relatively small from the linear line $y=x$ on the XY plot of the measured values vs. the predictive values. Value of ≥ 0.8 as the R^2 is recommended.

5) t value check → Recalculation



- Return to the [Execution of Regression Analysis] window, and check if the absolute value of t for each component term is low (<2) or not. $|t|$ value is recommended to be ≥ 2 .
- In this example, $|t|$ of Fe_2O_3 , As_2O_3 and Sb_2O_3 are <2 . First, delete $\checkmark$ in the checkboxes of As_2O_3 and Sb_2O_3 with $|t| < 1$, and recalculate. Second, delete $\checkmark$ in the checkbox of Fe_2O_3 with $|t| < 2$, and recalculate. By these procedures the component terms with $|t| < 2$ are removed from the multiple regression equation.



- Verification of the multiple regression analysis is performed again. R^2 decreases a little, but it is still high (0.98).

6) Completion of an additivity equation (multiple regression equation)

- The equation and the coefficients of its component terms are shown in the [Execution of Regression Analysis] window and the [Verification of Regression Analysis] window

- The obtained equation:

$$\text{Density at RT (g/cm}^3\text{)} = 2.273 \times (\text{SiO}_2) + 2.051 \times (\text{B}_2\text{O}_3) + 2.503 \times (\text{Al}_2\text{O}_3) + \dots\dots$$

(SiO₂), (B₂O₃), : mole ratio of each component (20 components except others)

- The analysis results can be saved in the user's PC from the [Save] icon in the [Data List for Regression Analysis] window. The save is available in the cases of Standard edition and CD Full Function edition, but not Internet edition.

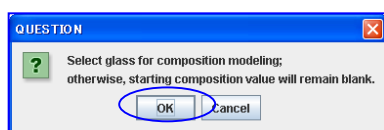
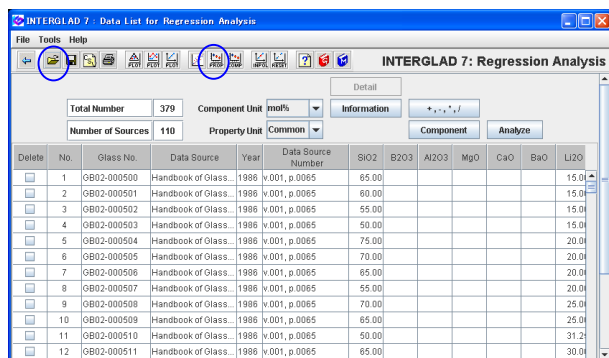
3.2 Property prediction — Density of zinc-silicate glasses

Predict density at RT of a glass with SiO₂ 60%, Li₂O 20% and ZnO 20% (mol%).

<Refer to D.2 of Chapter 3, 4.6 of Chapter 4>

The multiple regression equation obtained in 3.1 is used because of the same zinc-silicate glass system.

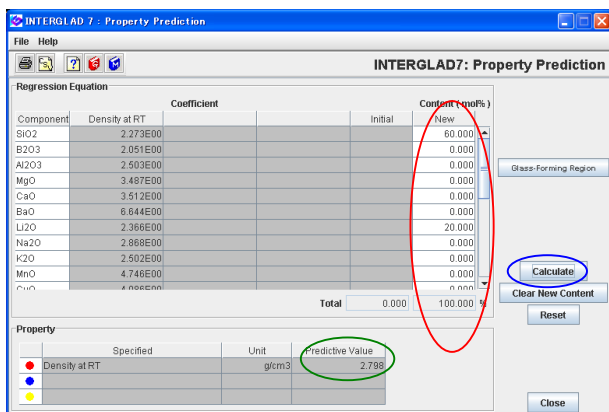
1) Regression analysis result → Transit to the [Property Prediction] window



- Open a [Data List for Regression Analysis] window, and by clicking the [Open] icon open the [Data List for Regression Analysis] window of the result of 3.1 saved in the folder of the user's PC.

- Here do not select any glass row. By clicking the [PROP] icon, a [Question] dialog box appears. Click the [OK] button, and the [Property Prediction] window opens.

2) Calculation of a property value



- Enter the specified component values of the composition to predict a property value in the [New] cells of the [Content] column. By clicking the [Calculate] button, the calculated value appears in the [Predictive Value] cell of the [Property] column.

- The predicted density: 2.798 g/cm³.

3.3 Composition optimization — Zinc-silicate glass with a specified density

Obtain a composition of zinc-silicate glass with 2.6 g/cm³ of density at RT. The components of the glass are SiO₂, B₂O₃, Na₂O, and ZnO.

<Refer to D.3 of Chapter 3, 4.7 of Chapter 4>

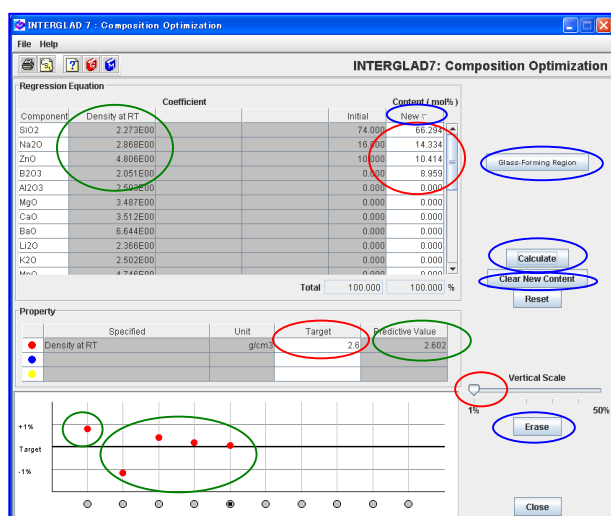
The multiple regression equation obtained in 3.1 is used because of the same zinc-silicate glass system.

1) Regression analysis result → Transit to the [Composition Optimization] window

No.	Glass No.	O3	La2O3	TiO2	ZrO2	P2O5	Nb2O5	Density at RT (g/cm3)	Density at RT (Predictive Value)	Density at RT (Residual)
172	GJ02-871993							2.5	2.612	-1.170E-1
288	GB07-174739							2.6	2.602	-2.410E-1
344	GJ02-191766R							2.6	2.544	-5.578E-1
45	GB02-000930							2.61	2.676	-6.579E-1
165	GJ02-062095							2.61	2.622	-1.153E-1
211	GC07-098731							2.61		
159	GC07-052393							2.62		
222	GB07-099544							2.62	2.685	-6.534E-1
340	GJ07-191722R							2.62	2.706	-8.815E-1
351	GJ02-191865R			2.35		0.27		2.62	2.675	-5.515E-1
29	GB02-000769							2.624	2.608	1.597E-1
353	GJ02-191867R			2.84		0.28		2.63	2.659	-2.886E-1

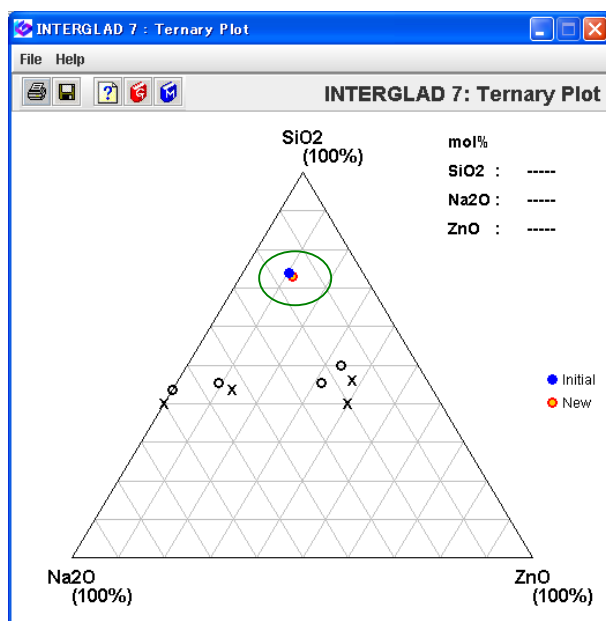
- Open a [Data List for Regression Analysis] window, and by clicking the [Open] icon open the [Data List for Regression Analysis] window of the result of 3.1 saved in the folder of the user's PC.
- Select a model glass which has a near density value to the target and which contains components of the target glass as possible by clicking the glass row. In this example sort the [Density at RT] column in the ascending order, and select a glass, No.165 (GJ02-062095) with 2.61 g/cm³ of density as a model.
- By clicking the [COMP] icon, the [Composition Optimization] window opens.

2) Composition optimization



- Enter the target value 2.6 in the [Target] cell of the [Property] column, and click the [Calculate] button. The calculated value appears in the [Predictive Value] cell. In the graph on the bottom part of the window, the difference between the value of the model glass and the target is shown as a point in red color. Drag the slider of the [Vertical Scale] to the left 1%, and the difference is magnified for easy visualization.

- By clicking the [Clear New Content] button, the values in the [New] cells become null. Enter component values in the [New] cells of SiO₂, B₂O₃, Na₂O and ZnO referring the initial (model) values. In this example enter the close integral numbers of the initial values for SiO₂, B₂O₃ and ZnO, and 10 for B₂O₃. Here sort the [New] column in descending order for checking.
 - By clicking the [Calculate] button, the property value is calculated after the proportional conversion of total values of components to 100%, and it appears in the [Predictive Value] cell. At the same time a new red point appears also in the graph, and the difference between the calculated value and the target value can be checked.
 - Next correct the values in the [New] column, and recalculate. Repeat these procedures to bring the calculated value close to the target value. When the red point becomes apart from the target, click the [Erase] button to cancel the predictive value, and the red point and the composition return to the previous state. Component terms with a higher absolute value of regression coefficient have higher effect on the increase or decrease of the property value. In this example, increase content of ZnO with a high coefficient little by little.
 - In final the Density at RT becomes 2.602 g/cm³ in case of the following composition.
The composition: SiO₂ 66.3%, B₂O₃ 9.0%, Na₂O 14.3%, and ZnO 10.4% (mol%).
 - The composition with the target property is not only one. So fix the values of components with some limitation, calculate changing the other components, and optimize the composition.
- 3) Investigation of relation between glass-forming region of ternary system and the predicted data



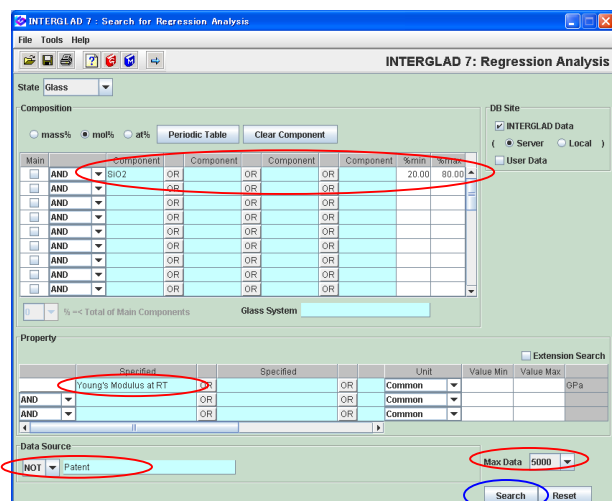
- By using the [Glass-Forming Region] button, the [New] and [Initial] composition can be shown in the [Ternary Plot] window. In this example the [Initial] and [New] compositions are plotted with the glass-forming region data of SiO₂-Na₂O-ZnO system.
- Glass-forming region data of the Ternary Plot are those where the sum of 3 components is 100%. So note that the difference increases as the other components besides the 3 components increase.

3.4 Property prediction by a linear equation — Young's modulus of alkaline-earth silicate glasses

Predict Young's modulus at RT of alkaline-earth silicate glasses with the composition of SiO₂ 45%, Al₂O₃ 12%, MgO 13%, CaO 20%, Y₂O₃ 7% and TiO₂ 3% (mol%).

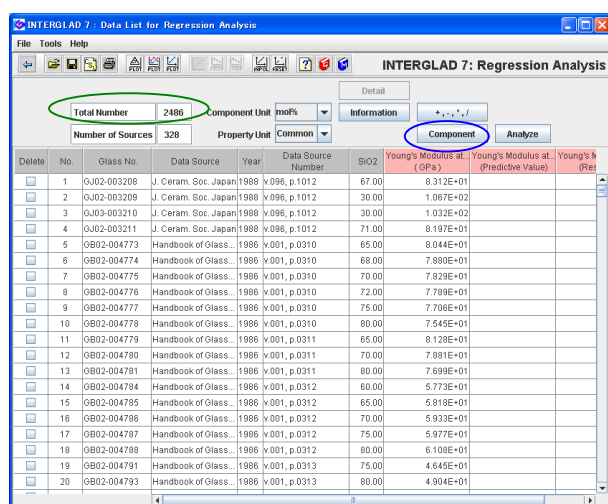
<Refer to D.2 of Chapter 3, 4.2-4.6 of Chapter 4>

1) Specification of search conditions ([Search for Regression Analysis] window) → Search



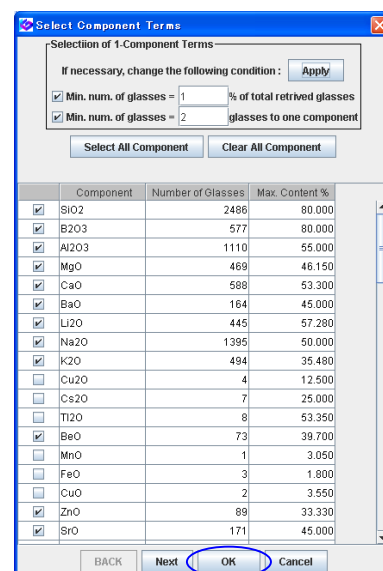
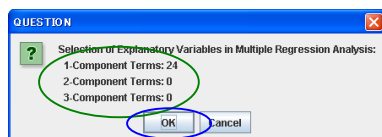
- Specify $20 \leq \text{SiO}_2 \leq 80 \text{ mol\%}$ for the Composition. Select 'Young' Modulus at RT' for the Property, and 'NOT Patent' for the Data Source. Various search conditions for the composition are available in this example. Here a simple composition condition by which many data can be collected is selected.

2) Search result ([Data List for Regression Analysis] window) → Selection of explanatory variables ([Selection of 1, 2, 3-Component Terms] dialog boxes)

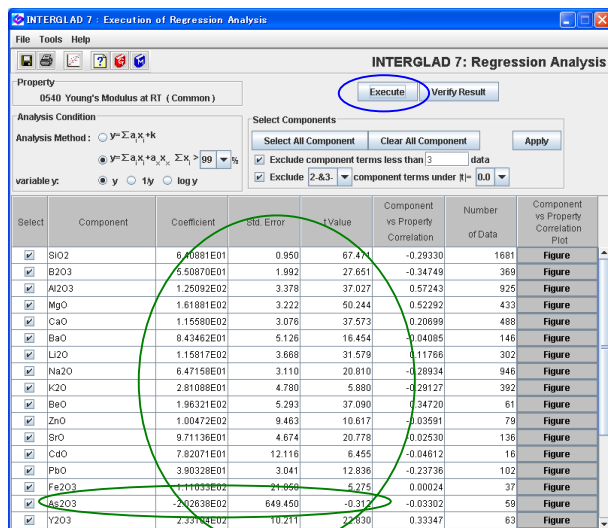


- 2486 glasses are listed.
- Specify only 1-component terms for explanatory variables at default setting.

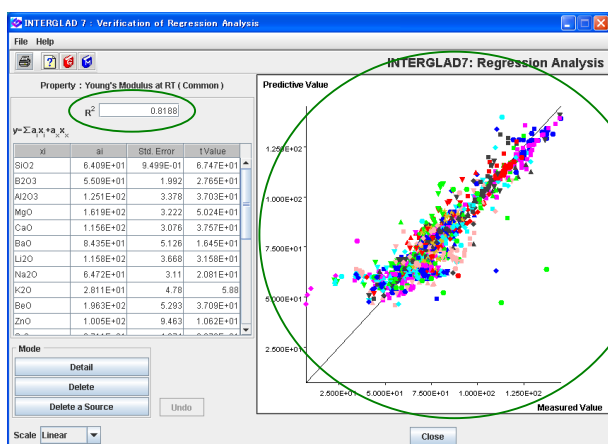
1-component terms: 24.



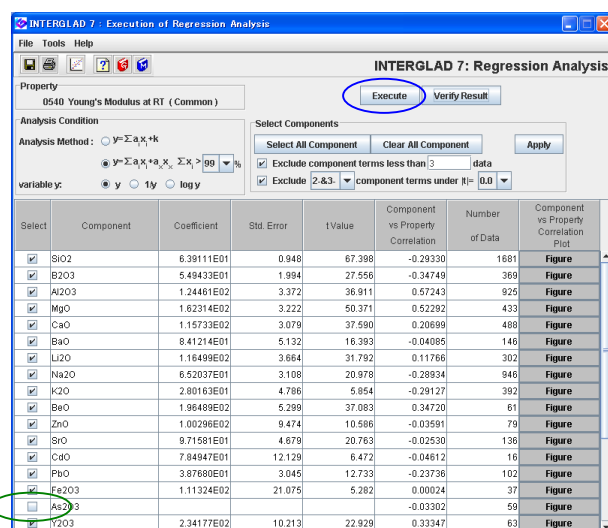
3) Execution of regression analysis ([Execution of Regression Analysis] window → [Verification of Regression Analysis] window)



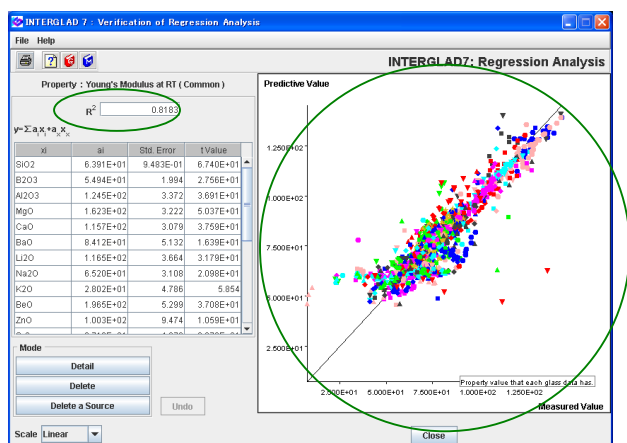
- In the [Execution of Regression Analysis] window, click the [Execute] button. Click the [OK] button in each [Question] dialog box which appears one after another. Finally the regression coefficients, etc. are shown.



- Open the [Verification of Regression Analysis] window by clicking the [Verify Result] button. The contribution rate R^2 is 0.8188. A lot of plot-points concentrate near a line of $y = x$. If recalculation is performed after deleting separate plot-points, R^2 will increase, but the effect on the regression equation would be small. In this example a simple prediction is performed without such a data delete.

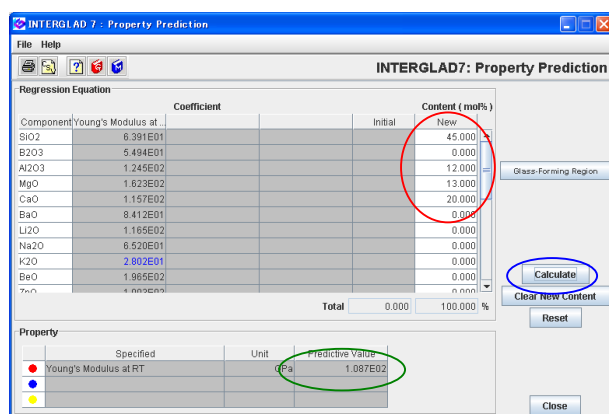


- $|t|$ of As_2O_3 is 0.312, which is ≤ 2 . Delete ☒ in the checkbox of As_2O_3 , and click the [Execute] button again.



- In this case R^2 is 0.8183 (≥ 0.8).
- $|t|$ value of each component term becomes ≥ 2 . The multiple regression equation is completed.

4) Property prediction ([Property Prediction] window)



- Return to the [Data List for Regression Analysis] window, and without selecting any glass, click the [PROP] icon. In the opened [Question] dialog box, click the [OK] button, and the [Property Prediction] window opens.
- Enter the specified component values (SiO₂ 45%, Al₂O₃ 12%, MgO 13%, CaO 20%, Y₂O₃ 7%, TiO₂ 3%) in the [New] cells, and click the [Calculate] button.
- 108.7 GPa for Young's modulus appears in the [Predictive Value] cell of the [Property] column.

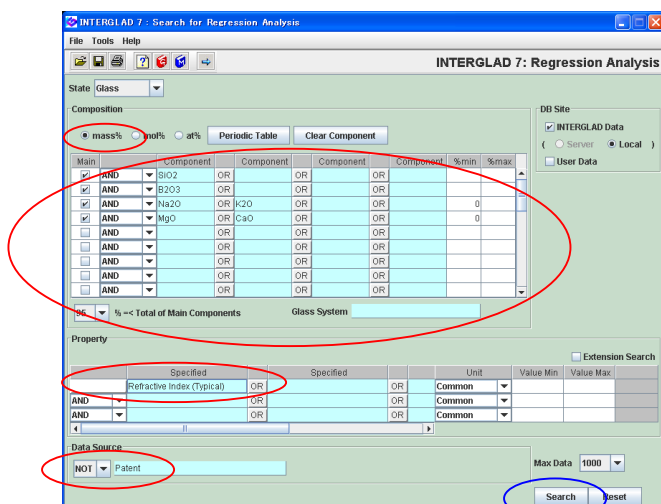
3.5 Property prediction by a cubic equation – Refraction index of boro-silicate glasses

Predict refraction index of glasses of $\text{SiO}_2\text{-B}_2\text{O}_3\text{-R}_2\text{O-RO}$ system with the following composition.

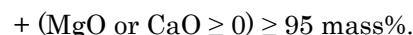
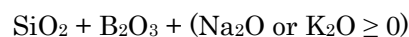
SiO_2 65%, B_2O_3 10%, MgO 5%, CaO 4%, Na_2O 7%, K_2O 5%, Al_2O_3 4% (mass%).

<Refer to D.2 of Chapter 3, 4.2-4.6 of Chapter 4>

1) Specification of search conditions ([Search for Regression Analysis] window) → Search



- Specify the following condition of composition.



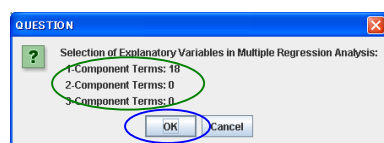
- Select 'Refractive Index (Typical)' for the Property, and 'NOT Patent' for the Data Source.

2) Search result ([Data List for Regression Analysis] window)

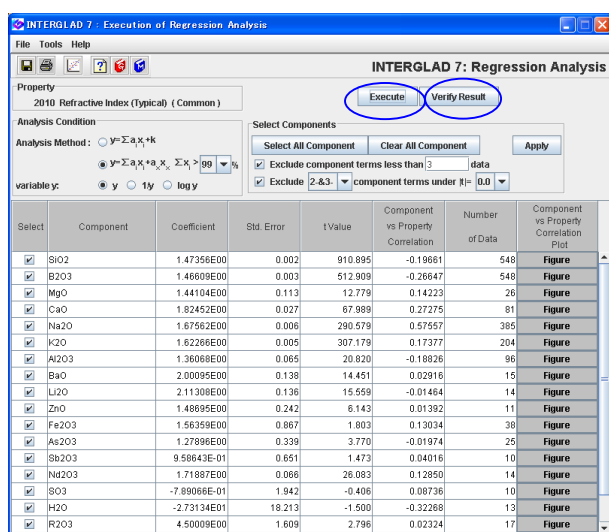
Delete	No.	Glass No.	Data Source	Year	Data Source Number	SiO2	B2O3	MgO	CaO	Na2O	K2O	Refractive
☐	1	QJ05-008626	Glastech. Ber.	1987	v.060, p.0234	73.03	16.92			10.04		
☐	2	QJ05-008627	Glastech. Ber.	1987	v.060, p.0234	72.65	16.93			9.99	1.52	
☐	3	QJ05-008628	Glastech. Ber.	1987	v.060, p.0234	71.91	16.66			6.92	4.51	
☐	4	QJ05-008629	Glastech. Ber.	1987	v.060, p.0234	71.54	16.58			5.90	5.98	
☐	5	QJ05-008630	Glastech. Ber.	1987	v.060, p.0234	71.17	16.49			4.89	7.44	1.502
☐	6	QJ05-008631	Glastech. Ber.	1987	v.060, p.0234	70.81	16.41			3.89	8.88	
☐	7	QJ05-008632	Glastech. Ber.	1987	v.060, p.0234	70.46	16.33			2.91	10.31	
☐	8	QJ05-008633	Glastech. Ber.	1987	v.060, p.0234	69.75	16.16			0.96	13.12	
☐	9	QJ05-008634	Glastech. Ber.	1987	v.060, p.0234	69.41	16.08					
☐	10	OB05-010781	Handbook of Glass...	1986	v.001, p.0548	84.69	15.31					
☐	11	OB05-010782	Handbook of Glass...	1986	v.001, p.0548	83.81	16.19					
☐	12	OB05-010783	Handbook of Glass...	1986	v.001, p.0548	77.54	22.46					
☐	13	OB05-010784	Handbook of Glass...	1986	v.001, p.0548	64.71	35.28					
☐	14	OB05-010785	Handbook of Glass...	1986	v.001, p.0548	63.32	36.68					
☐	15	OB05-010786	Handbook of Glass...	1986	v.001, p.0548	4.99	95.01					
☐	16	OB05-010787	Handbook of Glass...	1986	v.001, p.0548	84.69	15.31					
☐	17	OB05-010786	Handbook of Glass...	1986	v.001, p.0549	57.15	42.83					
☐	18	OB05-010797	Handbook of Glass...	1986	v.001, p.0549	51.76	48.22					
☐	19	OB05-010798	Handbook of Glass...	1986	v.001, p.0549	44.72	55.26					
☐	20	OB05-010799	Handbook of Glass...	1986	v.001, p.0549	40.01	59.98					

- 740 glasses are listed.
- First, regression analysis by a linear equation is carried out for comparison.
- In case of selection of only 1-component terms at default setting, 18 component terms are selected.

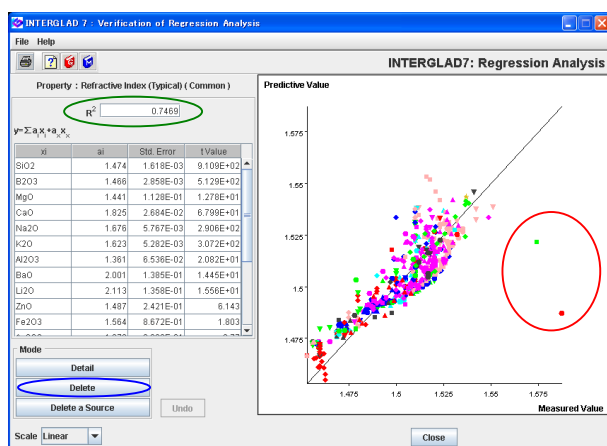
3) Regression analysis by a linear equation



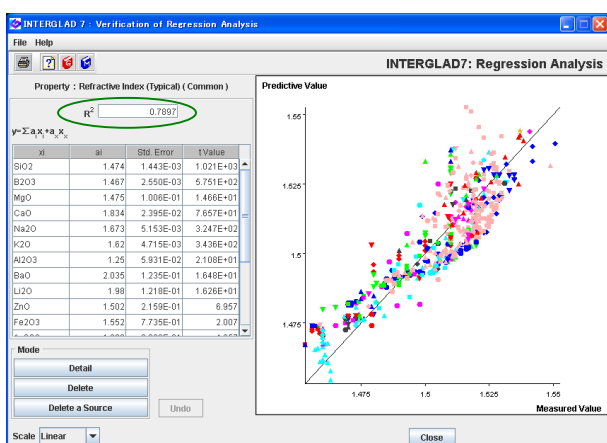
Component	Number of Glasses	Max. Content %
☒ SiO2	740	97.440
☒ B2O3	740	98.080
☒ MgO	27	5.500
☒ CaO	84	16.000
☒ Na2O	532	39.910
☒ K2O	221	42.940
☒ Al2O3	109	5.000
☒ BaO	15	3.000
☒ Li2O	16	4.960
☐ MnO	1	0.004
☐ FeO	2	0.085
☐ CoO	4	0.370
☐ NiO	4	0.370
☒ ZnO	12	3.000
☐ PbO	2	0.420
☒ Fe2O3	41	0.660
☒ As2O3	28	1.700
☒ Sb2O3	10	1.200



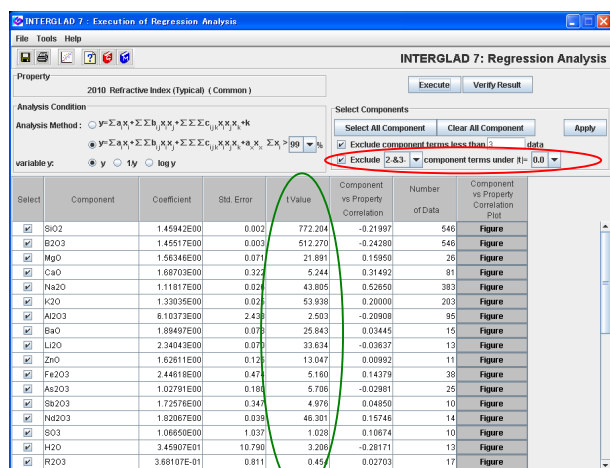
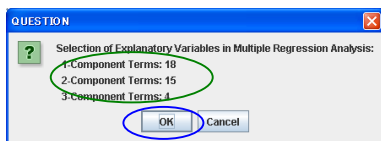
- Execute the regression analysis in the [Execution of Regression Analysis] window, and open the [Verification of Regression Analysis] window. The contribution rate R^2 is relatively low, 0.7469, and the plot-points have some difference from $y=x$.



- After removing 2 separated plot-points from $y=x$, execute the regression analysis again. The obtained R^2 is still low, 0.7897. So this linear regression equation is not sufficient for good prediction.



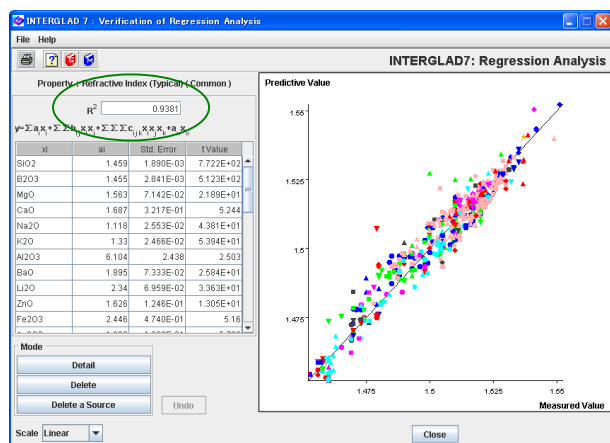
4) Regression analysis by a cubic equation



- Return to the [Data List for Regression Analysis] window, and select the 1, 2, 3-component terms at default setting. The numbers of the selected component terms are shown in the [Question] dialog box.

- Execute the regression analysis in the [Execution of Regression Analysis] window, and open the [Verification of Regression Analysis] window. R^2 is found to be 0.9381, a good result.

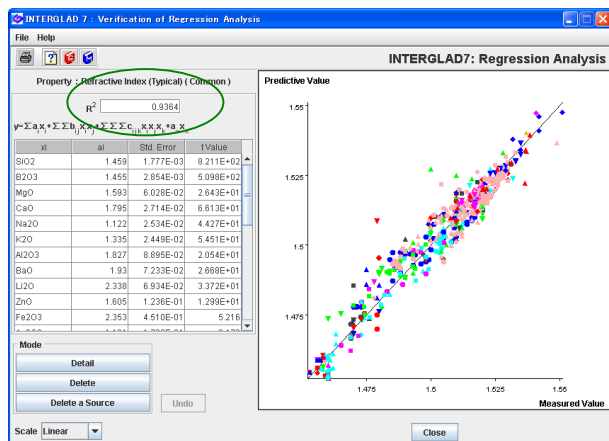
- Check t values in the [Execution of Regression Analysis] window. Component terms with $|t| < 2$ are 11 (1-component terms: 2, 2-component terms: 8, 3-component terms: 1).



- In the third row of the [Select Components] column, set up an excluding condition of component terms with low $|t|$ values, click the [Apply] button, and click the [Execute] button. Exclude not in one time, step by step as follows.

- Exclude '2 & 3' component terms under $|t| = '1.0.'$
- Exclude '2 & 3' component terms under $|t| = '2.0.'$
- Exclude 'all' component terms under $|t| = '1.0.'$
- Exclude 'all' component terms under $|t| = '2.0.'$

Finally all the $|t|$ values become ≥ 2.0 , and $R^2 = 0.9364$.



5) Property prediction ([Property Prediction] window)

- Return to the [Data List for Regression Analysis] window, and open the [Property Prediction] window from the [PROP] icon.
- Enter component values (SiO₂ 65%, B₂O₃ 10%, MgO 5%, CaO 4%, Na₂O 7%, K₂O 5% Al₂O₃ 4%) in the [New] cells of the [Regression Equation/ Content] column, and click the [Calculate] button.
- 1.512 for the calculated refractive index value appears in the [Predictive Value] cell of the [Property] column.

3.6 Composition optimization by linear equations — Soda aluminosilicate glass with specified properties

Optimize composition of soda aluminosilicate glass with $80 \times 10^{-7}/^{\circ}\text{C}$ of thermal expansion coefficient and 1.49 of refractive index.

< Refer to D.3 of Chapter 3, 4.2-4.5 and 4.7 of Chapter 4 >

1) Specification of search conditions ([Search for Regression Analysis] window) → Search

- Specify a wide composition condition to collect many related data. For example set up composition conditions as follows.
 $10 \leq \text{SiO}_2 \leq 90\%$, $1 \leq \text{Al}_2\text{O}_3 \leq 25\%$,
 $1 \leq \text{Na}_2\text{O} \leq 25\%$, $\text{SiO}_2 + \text{Al}_2\text{O}_3 + \text{Na}_2\text{O} \geq 90\%$ (mass%).
- Select 'Expansion Coeff (Typical)' and 'Refractive Index (Typical)' for the Property. Specifying properties with 'Typical' is effective to collect many data.
- Select 'NOT Patent' for the Data Source in this example.

2) Search result ([Data List for Regression Analysis] window)

INTERGLAD 7: Regression Analysis

Total Number: 43
Number of Sources: 18

Delete	No.	Glass No.	Data Source	Year	Data Source Number	SiO2	Al2O3	Na2O	Expansion Coeff. (10 ⁻⁶ /K)	Expansion Co. (Predictive)
☐	1	QJ02-015829	J. Non-Crystalline S.	1977	v.026, p.0517	75.69	1.15	13.67	7.900E+01	
☐	2	QJ02-032267	J. Austral. Ceramic	1984	v.020, p.0053	74.57	1.56	14.22	8.690E+01	
☐	3	QJ02-032270	J. Austral. Ceramic	1984	v.020, p.0053	73.67	1.56	14.92	8.960E+01	
☐	4	QJ02-032271	J. Austral. Ceramic	1984	v.020, p.0053	73.46	1.56	15.13	9.050E+01	
☐	5	QJ02-032272	J. Austral. Ceramic	1984	v.020, p.0053	73.36	1.56	15.43	9.140E+01	
☐	6	OC05-051160	Schott AG (DE)		8329	84.00	3.00	3.00	2.750E+01	
☐	7	OC02-051349	Corning Inc. (US)		0080	73.00	1.00	17.00	9.350E+01	
☐	8	OC02-051362	Corning Inc. (US)	1976	0317	61.00	17.00	13.00	8.800E+01	
☐	9	QJ06-055405	Glastech. Ber.	1980	v.053, p.0149	63.38	12.03	24.58	1.210E+02	
☐	10	QJ06-055406	Glastech. Ber.	1980	v.053, p.0149	62.04	15.69	22.26	1.090E+02	
☐	11	QJ06-055407	Glastech. Ber.	1980	v.053, p.0149	61.67	18.88	19.45	1.000E+02	
☐	12	QJ06-055408	Glastech. Ber.	1980	v.053, p.0149	60.36	23.08	16.55	9.200E+01	
☐	13	QJ06-055409	Glastech. Ber.	1980	v.053, p.0149	59.94	24.20	15.86	8.850E+01	
☐	14	QJ06-082265	Glass Phys. & Chem.	1982	v.008, p.0121	65.26	15.63	9.47	7.500E+01	
☐	15	QJ06-082266	Glass Phys. & Chem.	1982	v.008, p.0121	66.19	16.52	10.05	7.500E+01	
☐	16	QJ06-082267	Glass Phys. & Chem.	1982	v.008, p.0121	66.70	17.11	10.40	7.200E+01	
☐	17	QJ06-082268	Glass Phys. & Chem.	1982	v.008, p.0121	68.74	19.44	11.82	7.000E+01	
☐	18	OB02-088942	Technical Glasses	1961	v.001, p.0265	70.94	1.14	21.29	1.030E+02	
☐	19	OB02-088094	Properties of Glass	1954	v.001, p.0232	72.12	8.95	18.77	8.110E+01	
☐	20	OB02-088095	Properties of Glass	1954	v.001, p.0232	72.22	6.87	20.67	9.390E+01	

- 43 glasses are listed.

3) Regression analysis by a linear equation

Select Component Terms

If necessary, change the following condition:

☒ Min. num. of glasses = 1 % of total retrieved glasses

☒ Min. num. of glasses = 2 glasses to one component

Component	Number of Glasses	Max. Content %
☒ SiO2	43	84.110
☒ Al2O3	43	24.430
☒ Na2O	43	24.580
☒ B2O3	3	10.000
☒ MgO	7	4.000
☒ CaO	27	9.950
☐ BaO	1	1.940
☐ Li2O	5	3.390
☒ K2O	6	6.540
☒ BeO	4	9.310
☒ ZnO	2	6.080
☐ SrO	1	1.050
☐ Cr2O3	1	0.320
☒ Fe2O3	14	0.430
☐ Sb2O3	1	0.200
☒ TiO2	5	5.690
☒ SO3	3	0.250
☐ F	1	4.130

- Open the [Select Component Terms (1-Component Terms)] dialog box by clicking the [Component] button, and click the [OK] button at default setting.
- Check that the 1-component terms are 13, and click the [OK] button.

QUESTION

Selection of Explanatory Variables in Multiple Regression Analysis:

1. Component Terms: 13

2. Component Terms: 0

3. Component Terms: 0

INTERGLAD 7: Execution of Regression Analysis

Property: 2010 Refractive Index (Typical) (Common)

Analysis Condition: $y = \sum a_i x_i + k$

Analysis Method: $y = \sum a_i x_i + a_{i+1} x_{i+1} \dots \sum x_i > 99$ %

variable y: ☒ y ☐ 1/y ☐ log y

Select Components:

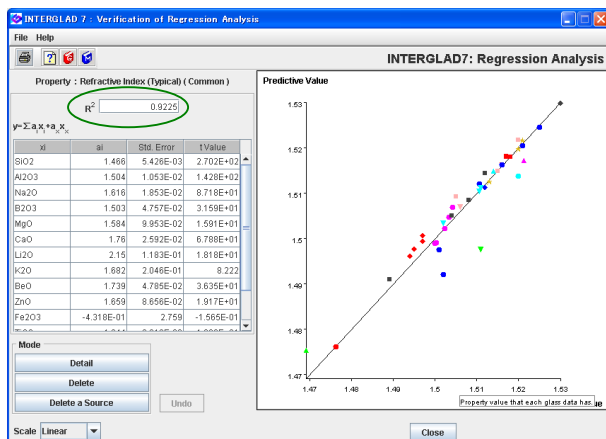
☒ Exclude component terms less than 3 data

☒ Exclude 2-43 component terms under 8

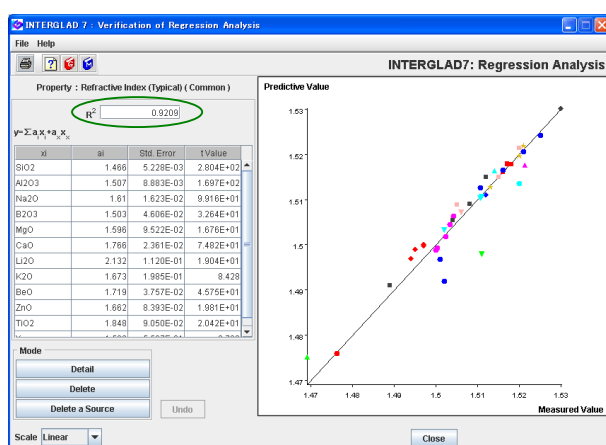
Select	Component	Coefficient	Std. Error	t-Value	Component vs Property Correlation	Number of Data	Component vs Property Correlation Plot
☒	SiO2	1.46602E00	0.005	270.165	-0.47664	43	Figure
☒	Al2O3	1.50377E00	0.011	142.807	0.12083	43	Figure
☒	Na2O	1.61568E00	0.019	87.177	0.24936	43	Figure
☒	B2O3	1.50262E00	0.048	31.585	-0.55167	3	Figure
☒	MgO	1.58360E00	0.100	15.911	0.06615	7	Figure
☒	CaO	1.75977E00	0.026	67.881	0.40293	27	Figure
☒	Li2O	2.15029E00	0.118	18.180	0.35606	5	Figure
☒	K2O	1.68227E00	0.205	8.222	-0.26234	6	Figure
☒	BeO	1.73941E00	0.048	36.353	0.30557	4	Figure
☒	ZnO	1.65908E00	0.087	19.168	0.14678	2	Figure
☒	Fe2O3	-4.31762E-01	2.759	-0.156	0.11591	14	Figure
☒	TiO2	1.84356E00	0.093	19.799	0.27654	5	Figure
☒	SO3	7.76641E00	8.536	0.910	0.06029	3	Figure
☐	xx	-3.18598E00	6.604	-0.482			

- After clicking the [Analyze] button in the [Data List for Regression Analysis] window, two [Execution of Regression Analysis] windows of refractive index and thermal expansion coefficient appear one upon another.
- First, click the [Execute] button in the window of refractive index. In each [Question] dialog box which appears one after another, click the [OK] button. Finally

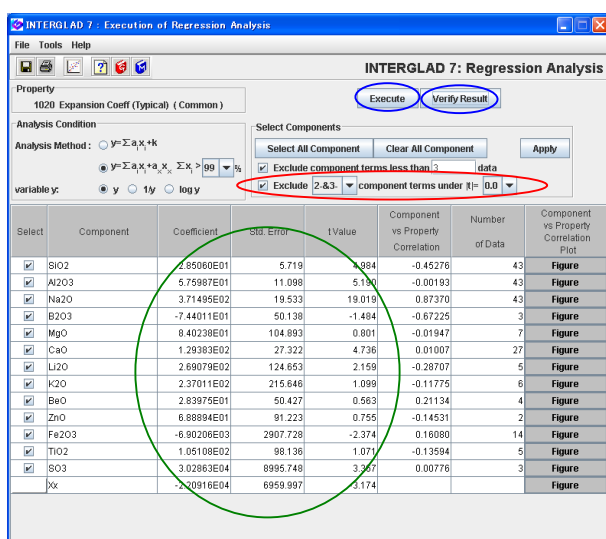
Coefficients, Std. Errors and t-Values appear in the table after the success of the calculation.



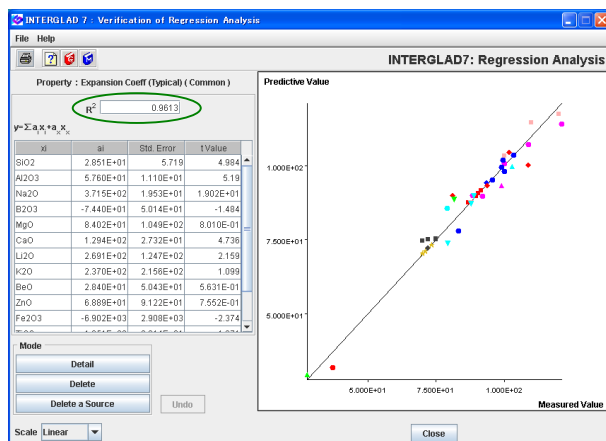
- Open the [Verification of Regression Analysis] window by clicking the [Verify Result] button.
- Note that the contribution factor R^2 is 0.9225, which is a good value over 0.9.
- Check t values. Component terms with $|t| < 2$ are 2.



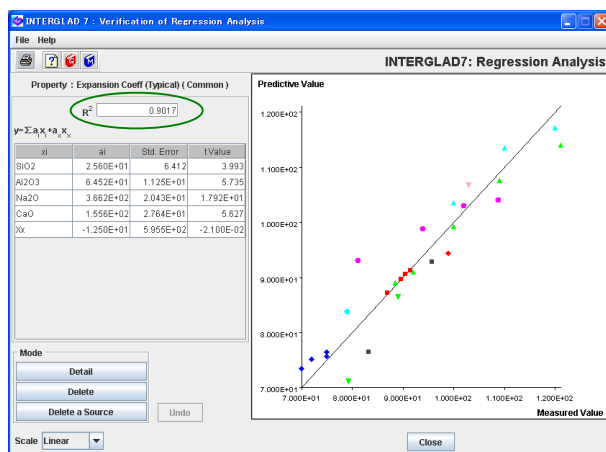
- Delete checks in the [Select] checkboxes of the component terms with low $|t|$ value, i.e. Fe_2O_3 with -0.156, SO_3 with 0.910, and execute again. Then all the $|t|$ values become ≥ 2 , and R^2 is 0.9209. By this operation the regression equation of refractive index is completed.



- Next execute the regression analysis in the [Execution of Regression Analysis] window of thermal expansion in the same manner.



- The obtained R^2 is 0.9613, sufficiently high.

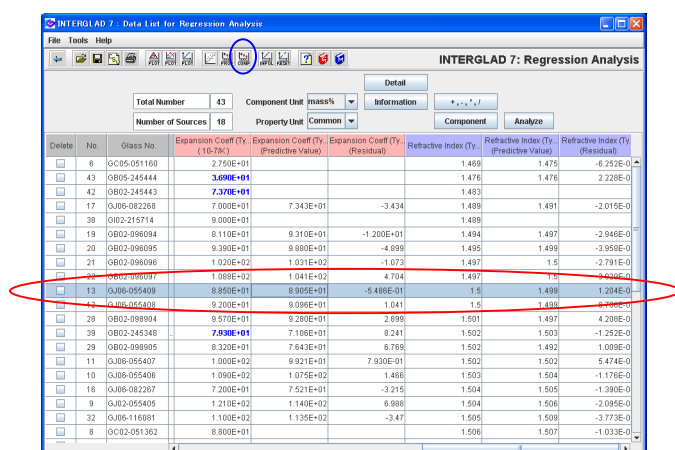


- In the third row of the [Select Component] column, set up an excluding condition of component terms with low $|t|$ values, click the [Apply] button, and click the [Execute] button in the following order.

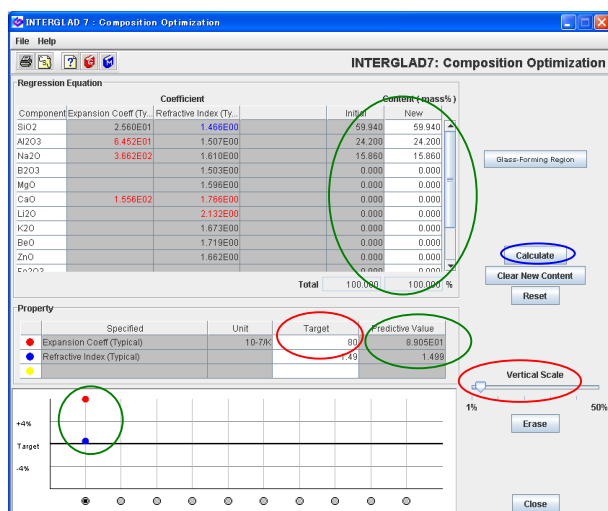
- Exclude 'all' component terms under $|t| = '1.0.'$
- Exclude 'all' component terms under $|t| = '1.0'$ again.
- Exclude 'all' component terms under $|t| = '1.5.'$

Finally all the $|t|$ values become ≥ 2.0 , and $R^2=0.9017$. The regression equation is completed.

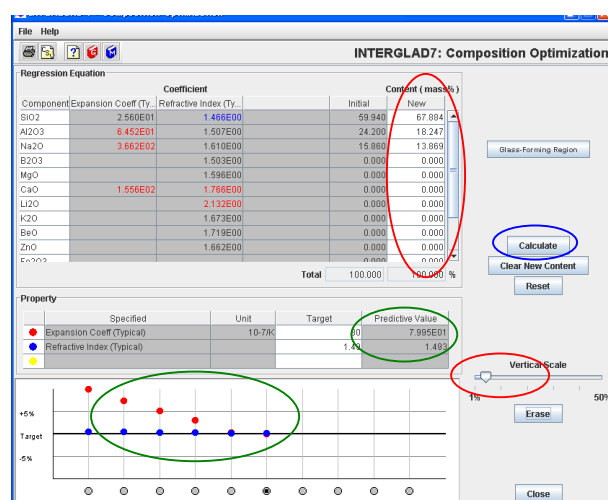
- Composition optimization([Data List for Regression Analysis] window → [Composition Optimization] window)



- Return to the [Data List for Regression Analysis] window, and select a glass with near properties to the target property. In this example select a glass row of No. 55409 in which the predictive value of Expansion Coeff is the nearest to the target value. Click the [COMP] icon, and open the [Composition Optimization] window.



- In the [Initial] and [New] cells of the [Regression Equation] column, the composition of No. 55409 appears.
- Enter the target values in the [Target] cells of the [Property] column.
Expansion Coeff (Typical): $80 \times 10^{-7}/^{\circ}\text{C}$.
Refractive Index (Typical): 1.49.
- By clicking the [Calculate] button, percentages of the predictive values divided by the target values respectively are shown in the graph.



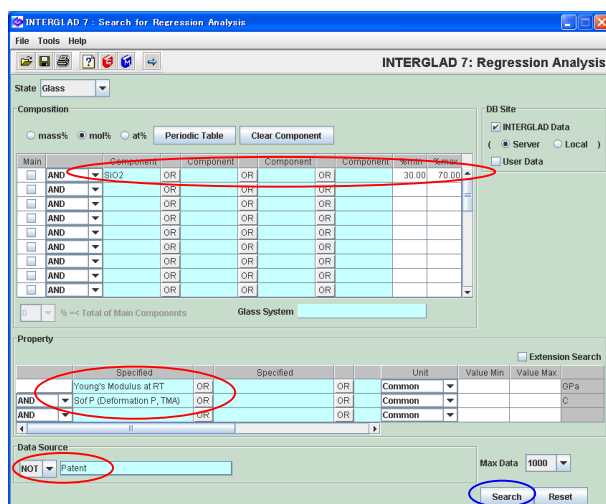
- By sliding the [Vertical Scale] to the left, the vertical scale of the graph is enlarged, and the user can easily check the difference between the target and predictive values.
- Enter component values in the [New] cells, click the [Calculate] button, and check the predictive values. Repeat these procedures to approximate the predictive values to the target values as possible.
- In this example the composition optimization is performed by increasing SiO₂ content and decreasing Al₂O₃ and Na₂O contents with high regression coefficients of thermal expansion.
- An optimized composition is as follows: SiO₂ 67.88%, Al₂O₃ 18.25%, Na₂O 13.87%. This glass has $79.95 \times 10^{-7}/^{\circ}\text{C}$ of thermal expansion coefficient and 1.493 of refractive index.

3.7 Composition optimization by cubic equations — Boro-silicate glass with specified properties

Design a composition of boro-silicate glass with 70 GPa of Young's modulus and 700°C of deformation point. The glass is composed of SiO_2 (30-70 mol%)- B_2O_3 - Al_2O_3 - CaO - BaO - Na_2O .

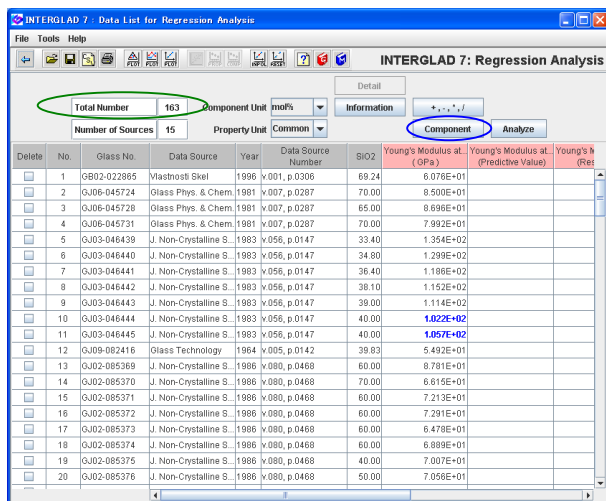
< Refer to D.3 of Chapter 3, 4.2-4.5 and 4.7 of Chapter 4 >

1) Specification of search conditions ([Search for Regression Analysis] window) → Search



- Select 'SiO2' for the Component, and enter 30% for the minimum and 70% for the maximum.
- Select 'Young's Modulus at RT' and 'Sof P (Deformation P, TMA)' for the Property.
- Select 'NOT Patent' for the Data Source.

2) Search result ([Data List for Regression Analysis] window)



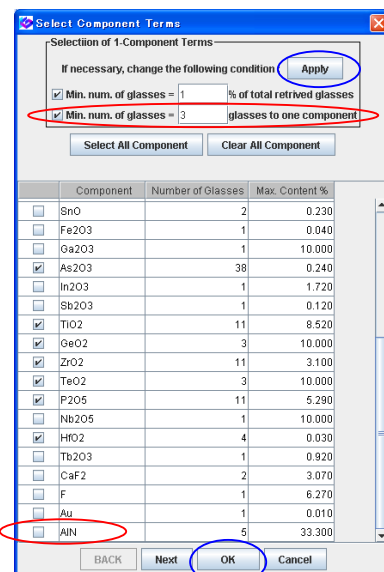
- 163 glasses are listed.

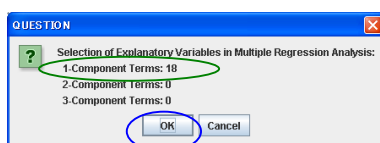
3) Regression analyses by linear equations

([Select Component Terms] dialog box

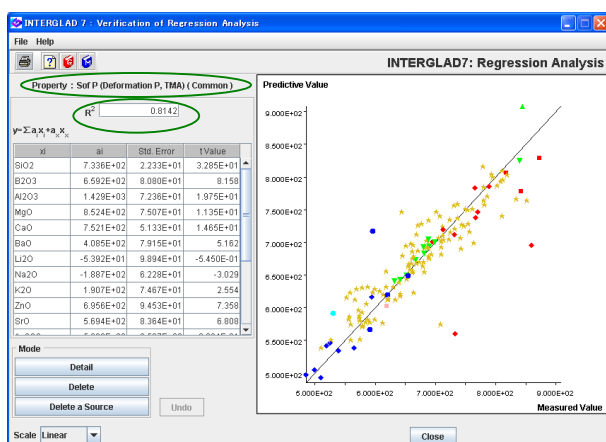
→ [Execution of Regression Analysis] window]

→ [Verification of Regression Analysis] window)

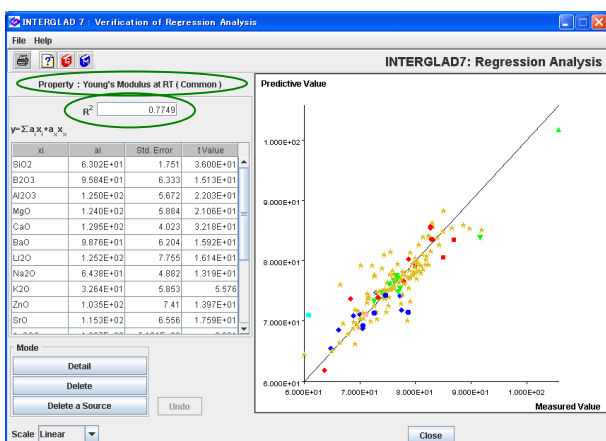




- In the [Select Component Terms (1-Component Terms)] dialog box, enter 3 for the minimum number of glasses that contain the component in the cell of the 3rd row, and click the [Apply] button. Delete check in the checkbox of AlN which is not oxide in the list.
- Note that 1-component terms are 18 in the [Question] dialog box.

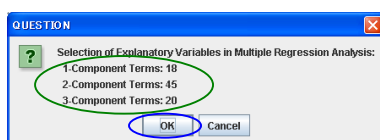


- In each [Execution of Regression Analysis] window of the 2 properties, execute the regression analysis at default setting, and verify the result in the [Verification of Regression Analysis] window.



- In the [Verification of Regression Analysis] window of deformation point, $R^2=0.8142$.
- In the [Verification of Regression Analysis] window of Young's modulus, $R^2=0.7749$.
- R^2 by linear equations for deformation point and Young's modulus are both ≤ 0.82 , not sufficiently high. So regression analyses by cubic equations are tried.
- Plot-points with yellow colored star in the graphs mean highly reliable 'Gold Data.' <Refer to 2.1 (2) (C) 2) of Chapter 4>
- Close the [Verification of Regression Analysis] windows and the [Execution of Regression Analysis] windows.

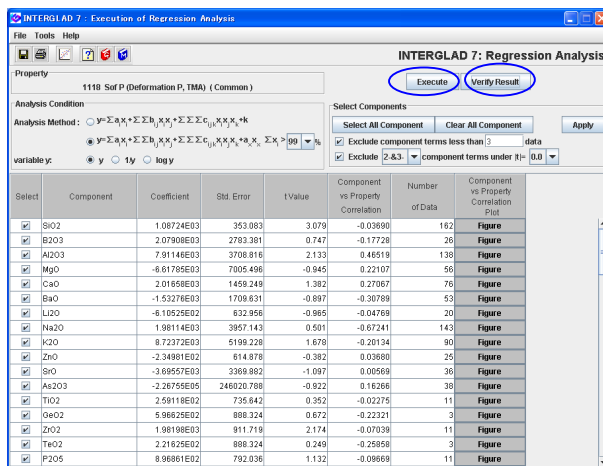
4) Regression analyses by cubic equations ([Select Component Terms] dialog box → [Execution of Regression Analysis] window) → [Verification of Regression Analysis] window)



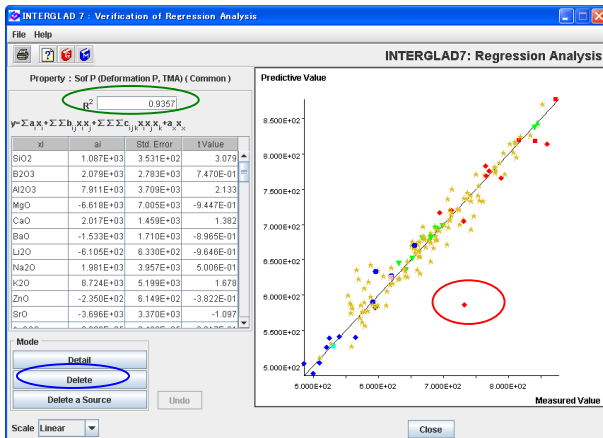
- In the [Data List for Regression Analysis] window, click the [Component] button, and open the [Select Component Terms] dialog

box.

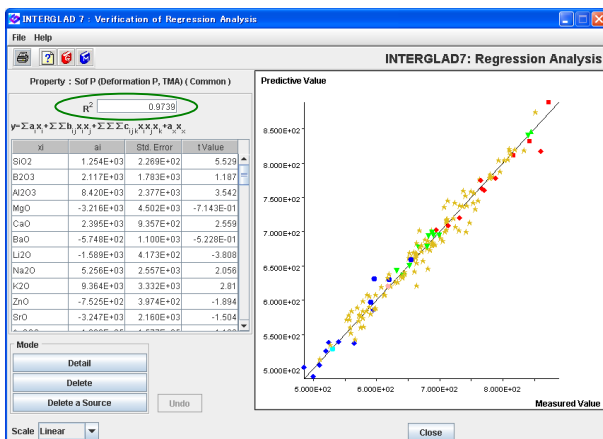
- Select the same 1-component terms as those for the linear equation, and 2, 3-component terms at default setting.
- 18 of 1-component terms, 45 of 2-component terms and 20 of 3-component terms are selected.



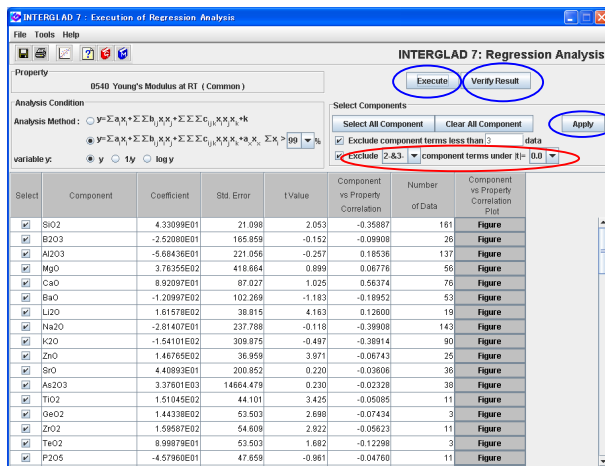
- In the [Execution of Regression Analysis] window of deformation point, execute the regression analysis.



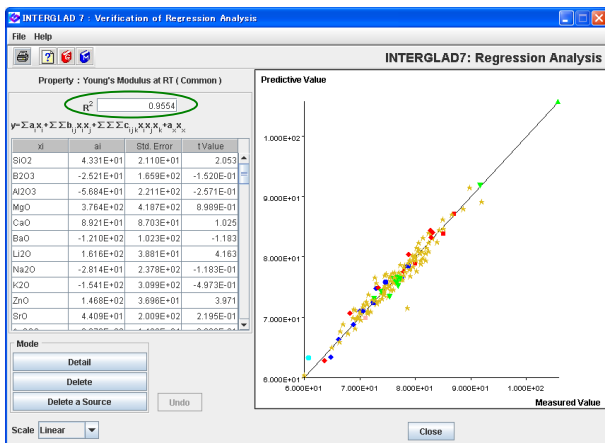
- In the [Verification of Regression Analysis] window, R^2 is 0.9357.
- Delete a separated plot-point from $y=x$ by clicking the plot-point after clicking the [Delete] button. Return to the [Execution of Regression Analysis] window, and click the [Execute] button to recalculate.



- As the result, R^2 increases to 0.9739.

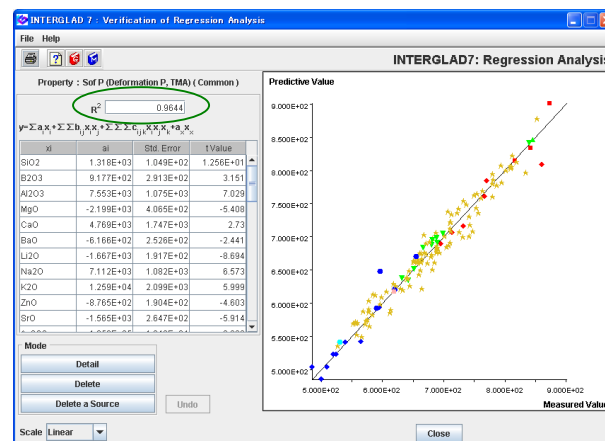


- Next, in the [Execution of Regression analysis] window of Young's modulus, Execute the regression analysis.



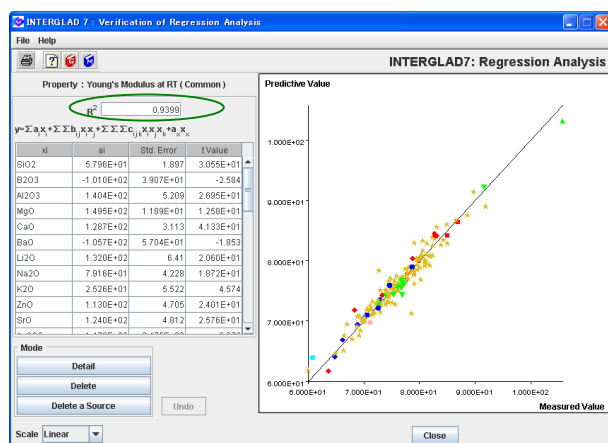
- R^2 is 0.9554 in the [Verification of Regression Analysis] window. No plot-point is separated largely from $y=x$

- Good results that R^2 for both properties are ≥ 0.9 are obtained. Then remove component terms which have low $|t|$ value.



- First in the [Execution of Regression Analysis] window of deformation point, set up an excluding condition of component terms with low $|t|$ values, click the [Apply] button and then [Execute] button in the following order.

- 1) Exclude '2-&3-' component terms under $|t| = '0.5.'$
- 2) Exclude '2-&3-' component terms under $|t| = '1.0'$ again.
- 3) Exclude '2-&3-' component terms under $|t| = '1.5.'$



4) Exclude 'all' component terms under $|t| = '0.5.'$

5) Exclude 'all' component terms under $|t| = '1.5.'$

6) Exclude '2-&3-' component terms under $|t| = '1.5.'$

After these procedures, the $|t|$ values are ≥ 1.4 for 1-component terms, ≥ 1.9 for 2-component terms, and ≥ 2.0 for 3-component terms. It is difficult to have a regression equation with $|t| \geq 2$ of all the component terms. Finally a regression equation with $R^2=0.9644$ is obtained.

- Next in the [Execution of Regression Analysis] window of Young's Modulus at RT, set up an excluding condition of component terms with low $|t|$ values, click the [Apply] button and then [Execute] button in the following order.

1) Exclude '2-&3-' component terms under $|t| = '0.5.'$ Perform this procedure 3 times.

2) Exclude '2-&3-' component terms under $|t| = '1.0.'$ Perform 2 times

3) Exclude '2-&3-' component terms under $|t| = '1.5.'$ Perform 2 times

4) Exclude '2-&3-' component terms under $|t| = '2.0.'$

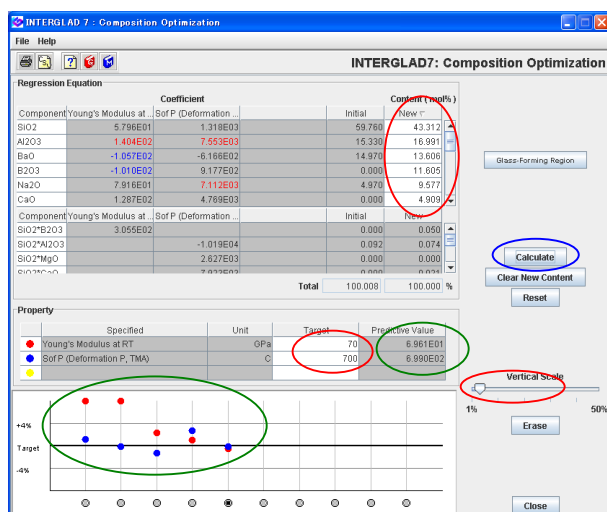
5) Exclude 'all' component terms under $|t| = '0.5.'$

After these procedures, the $|t|$ values are ≥ 1.9 for 1-component terms, ≥ 2.2 for 2-component terms, and ≥ 2.3 for 3-component terms. It is difficult to have a regression equation with $|t| \geq 2$ of all the component terms. Finally a regression equation with $R^2=0.9399$ is obtained.

5) Composition optimization([Data List for Regression Analysis] window → [Composition Optimization] window)

Delete	No.	Glass No.	Young's Modulus at (GPa)	Young's Modulus at (Predictive Value)	Young's Modulus at (Residual)	Sof P (Deformation) (C)	Sof P (Deformation) (Predictive Value)
☐	116	G103-191717	7.540E+01	7.441E+01	9.879E-01	6.900E+02	6.800E+02
☐	122	G106-191724R	7.220E+01	7.274E+01	-5.390E-01	6.770E+02	6.910E+02
☐	125	G103-191730	7.730E+01	7.619E+01	1.105	6.820E+02	6.949E+02
☐	108	G103-191708R	7.720E+01	7.611E+01	1.087	6.810E+02	6.979E+02
☐	115	G103-191716	7.660E+01	7.585E+01	7.498E-01	6.880E+02	6.987E+02
☐	81	G106-191674R	8.090E+01	8.019E+01	7.121E-01	7.310E+02	6.990E+02
☐	151	G102-191798R	7.050E+01	7.183E+01	-1.329	7.420E+02	7.002E+02
☐	117	G105-191719R	7.010E+01	6.979E+01	3.090E-01	7.010E+02	7.007E+02
☐	92	G106-191662R	8.180E+01	8.073E+01	1.166	6.800E+02	7.029E+02
☐	111	G103-191712	7.670E+01	7.540E+01	1.296	6.990E+02	7.046E+02
☐	107	G103-191708R	7.770E+01	7.774E+01	-4.485E-02	6.870E+02	7.054E+02
☐	88	G106-191667R	8.190E+01	7.919E+01	2.719	7.250E+02	7.064E+02
☐	84	G106-191680	8.310E+01	8.412E+01	-1.016	7.133E+02	7.074E+02
☐	126	G105-191745R	7.820E+01	7.884E+01	-6.374E-01	7.120E+02	7.094E+02
☐	76	G106-191668R	7.450E+01	7.663E+01	-2.123	7.470E+02	7.084E+02
☐	27	G102-190822R	7.200E+01	7.311E+01	-9.070E-01	7.100E+02	7.123E+02
☐	87	G106-191686	7.680E+01	8.042E+01	-1.62	7.320E+02	7.167E+02
☐	69	G106-191660R	7.890E+01	7.770E+01	1.189	7.430E+02	7.179E+02
☐	30	G106-190613R	7.798E+01	7.883E+01	-8.514E-01	7.100E+02	7.219E+02
☐	24	G106-190605R	8.232E+01	8.250E+01	-1.789E-01	7.120E+02	7.219E+02

- Return to the [Data List for Regression Analysis] window, and select a model glass with near properties to those of the target. Sort Sof P in ascending order in this example. Select a glass row of No. 196688R in which the predictive value of Sof P is 708°C and which contains BaO. Click the [COMP] icon, and open the [Composition Optimization] window.



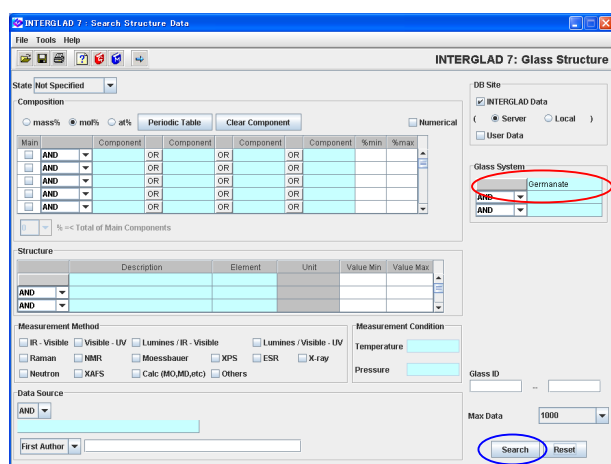
- Enter the target values, 70 GPa for Young's Modulus and 700°C for Sof P in the [Target] cells.
- After clicking the [Calculate] button, the predictive values of the model composition appear in the [Predictive Value] cells and the differences to the target values are shown in the graph.
- Enter values for necessary components with 0 and 0 for unnecessary components in the [New] cells referring the composition of the model glass. The operation becomes easy by sorting the [New] column.
- Repeat the calculation changing the composition and checking the differences to the target values in consideration of the values of the regression coefficients
- An optimized composition is as follows: SiO₂ 43.3%, B₂O₃ 11.6%, Al₂O₃ 17.0%, CaO 4.9%, BaO 13.6%, Na₂O 9.6% (mol%). This glass has 69.6 GPa of Young's modulus at RT and 699°C of softening (deformation) temperature.

4. Search and Analysis of Structure Data

4.1 Investigation of structure information – Germanate glasses

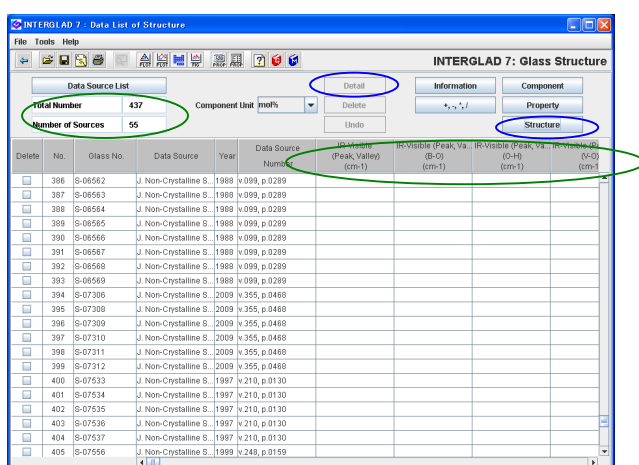
< Refer to E of Chapter 3, and 5 of Chapter 4 >

1) Specification of search conditions ([Search Structure Data] window) → Search

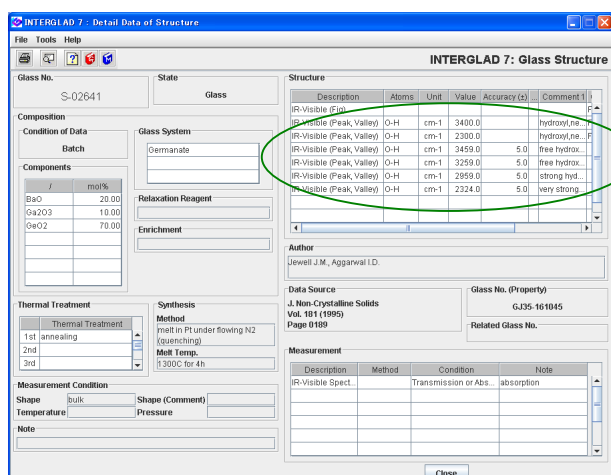


- Select 'Germanate' for the Glass System.

2) Search result ([Data List of Structure] window and the [Detail Data of Structure] window)



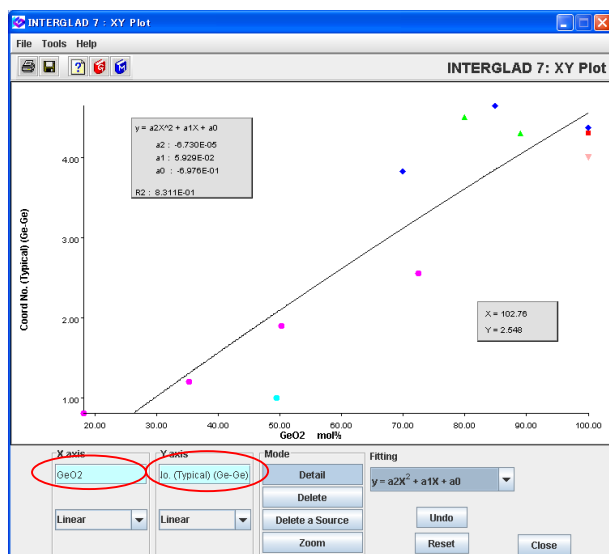
- 437 glasses of 55 data sources are listed.
- To know what kind of information is registered about the searched glasses, click the [Structure] button, and select the [Select All] button in the [Select Structure] dialog box.
- It is found that data of each glass are few but that more than 100 property items are registered in total. Below, several data are explained including some notices for use.



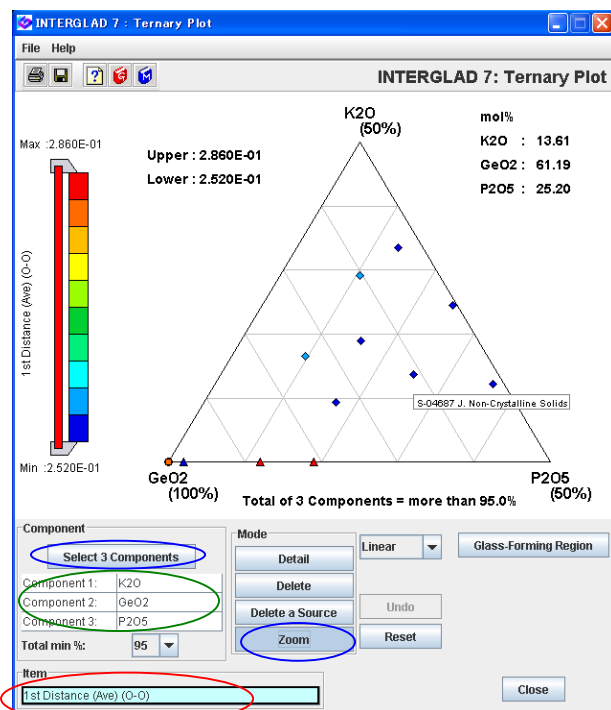
- The left figure is the [Detail Data of Structure] window of S-02641. 6 values of wave number for IR-Visible (Peak, Valley) (OH) are shown. In such a case only the first value is listed in the [Data List of Structure] window. In the Structure Database, check of the [Detail Data of Structure] window is

occasionally necessary because of the similar data registration in many glasses. Figures of spectroscopy are usually not stored in INTERGLAD.

3) Utilization of search result ([XY Plot] window and [Ternary Plot] window)



- The figure is an XY Plot of content of GeO_2 vs. coordination number (Ge-Ge). In this example 'Coord No. (Typical)' means 1st neighbour coordination number. With increasing the content of GeO_2 , coordination number of Ge around Ge increases.

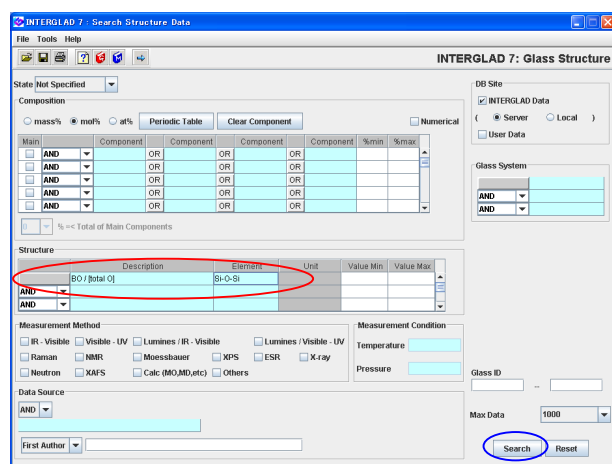


- The figure is an example of Ternary Plot, and it shows values of the 1st interatomic distance (O-O) with 10 colors in GeO_2 - P_2O_5 - K_2O system. This figure is a zoomed Ternary Plot of GeO_2 (100%) - P_2O_5 (50%) - K_2O (50%).

4.2 Investigation of correlation between composition and structure — SiO₂ content and bridging oxygen fraction

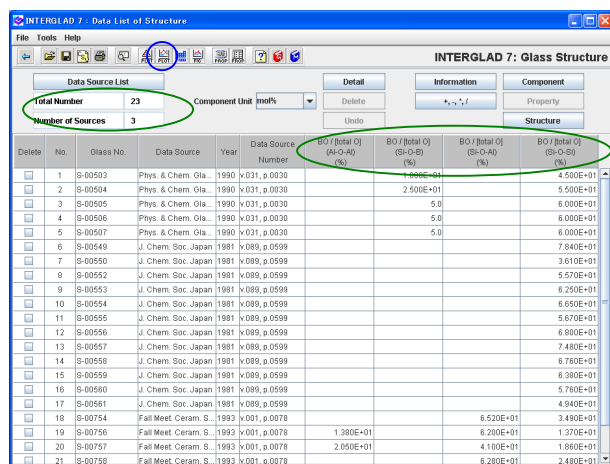
< Refer to E of Chapter 3, and 5 of Chapter 4 >

1) Specification of search conditions ([Search Structure Data] window) → Search



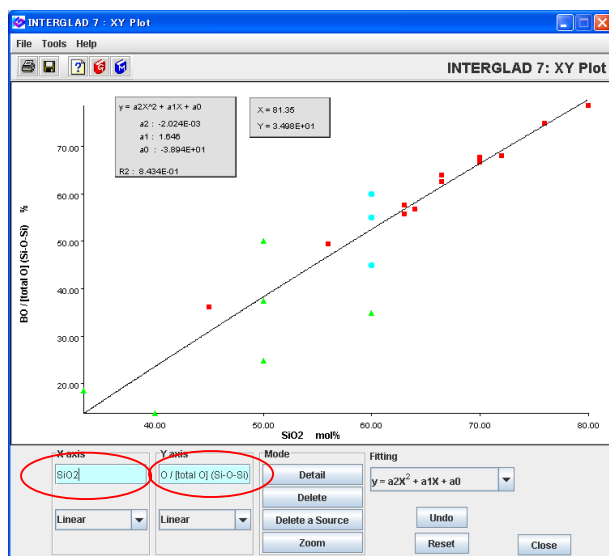
- Specify 'BO/[totalO]' for the Description, and Si-O-Si for the Element in the [Structure] column. 'BO/[totalO] (Si-O-Si)' means fraction of bridging oxygen with Si to the total oxygen.

2) Search result ([Data List of Structure] window)



- 23 glasses of 3 data sources are listed.
- BO/[totalO] data of not only Si-O-Si but also Al-O-Al, Si-O-B and Si-O-Al appear in the list.

3) Utilization of search result ([XY Plot] window)



- An XY plot of SiO₂ content vs. BO/[total O] (Si-O-Si) is shown.
- As composition is not specified in this example, various components are contained. It is found that the bridging oxygen increases with increasing SiO₂ content.

4.3 Investigation of correlation between structure factors — Q² and non-bridging oxygen fraction of alkali-silicate glasses

< Refer to E of Chapter 3, and 5 of Chapter 4 >

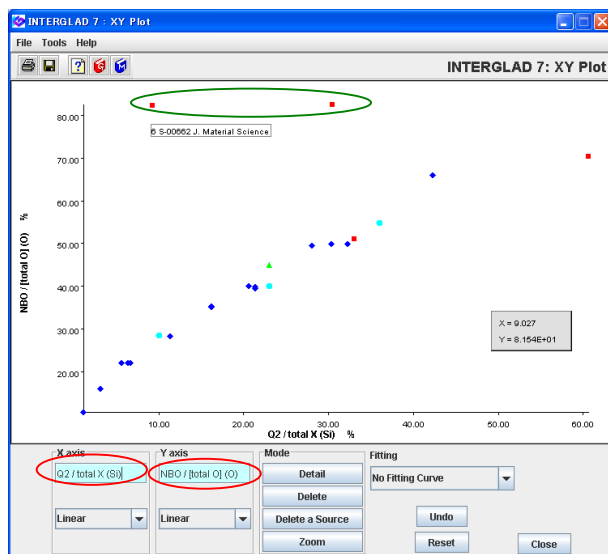
1) Specification of search conditions ([Search Structure Data] window) → Search

- Specify 'Alkali Silicate' for the Glass System. Select 'Q2/totalX' of the 'Qn Distribution' and 'NBO/[totalO]' both in the 'Bridging Oxygen Information' for the Description of the [Structure] column. 'Q2/totalX' means Q² fraction in tetrahedra XO₄. 'NBO/[totalO]' means fraction of non-bridging oxygen to the total oxygen.

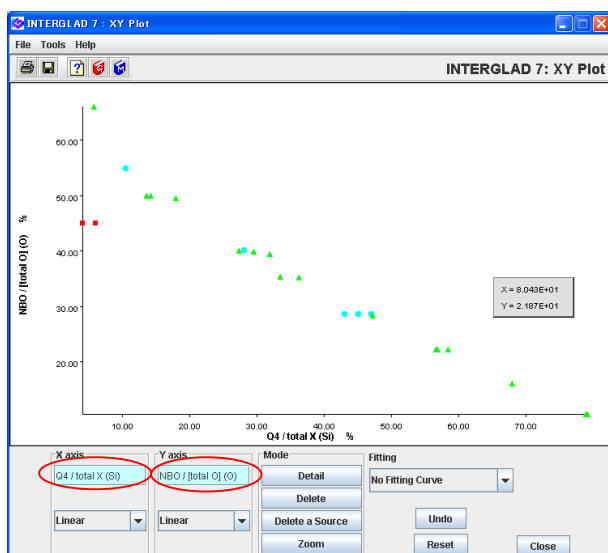
2) Search result ([Data List of Structure] window)

No.	Glass No.	Data Source	Year	Data Source Number	NBO/[total O] (O) (%)	NBO/[total O] (Si-O) (%)	NBO/[total O] (Ca-O) (%)	NBO/[total O] (Si)
1	S-00119	J. Non-Crystalline S.	2002	v.297, p.0220	2.880E+01			
2	S-00120	J. Non-Crystalline S.	2002	v.297, p.0220	4.010E+01			
3	S-00121	J. Non-Crystalline S.	2002	v.297, p.0220	5.480E+01			
4	S-00122	J. Non-Crystalline S.	2002	v.297, p.0220	2.860E+01			
5	S-00123	J. Non-Crystalline S.	2002	v.297, p.0220	2.860E+01			
6	S-00682	J. Material Science	1993	v.028, p.3473	8.220E+01			
7	S-00683	J. Material Science	1993	v.028, p.3473	8.220E+01			
8	S-00684	J. Material Science	1993	v.028, p.3473	7.030E+01			
9	S-00685	J. Material Science	1993	v.028, p.3473	5.110E+01			
10	S-01150	J. Jpn. Inst. Metals	1983	v.047, p.0382	4.500E+01			

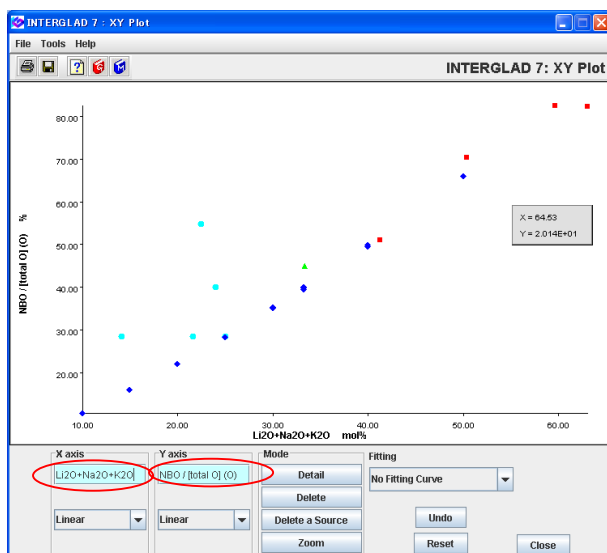
- 37 glasses of 5 data sources are listed.
- As NBO/[totalO], not only NBO/[totalO] (O) but also those of (Si-O) and (Ca-O) are listed. As Q²/totalX, Q²/totalX (Al) is also listed besides that of (Si).

3) Correlation between Q^2 and NBO ([XY Plot] window)

- An XY Plot of $Q^2/\text{totalX}(\text{Si})$ vs. $\text{NBO}/[\text{totalO}](\text{O})$ is shown.
- With increasing Q^2 , NBO fraction increases almost proportionally. When the 2 glasses at separated positions from the others are checked in the [Detail Data of Property] windows of the corresponding Glass No. (Property), it is found that they are both rapid-quenched glasses. This is the reason why the plot-points are separated from the others.



- For comparison, an XY Plot of $Q^4/\text{totalX}(\text{Si})$ vs. $\text{NBO}/[\text{totalO}](\text{O})$ is shown.
- The figure shows a reasonable tendency that NBO fraction decreases with increasing Q^4 .

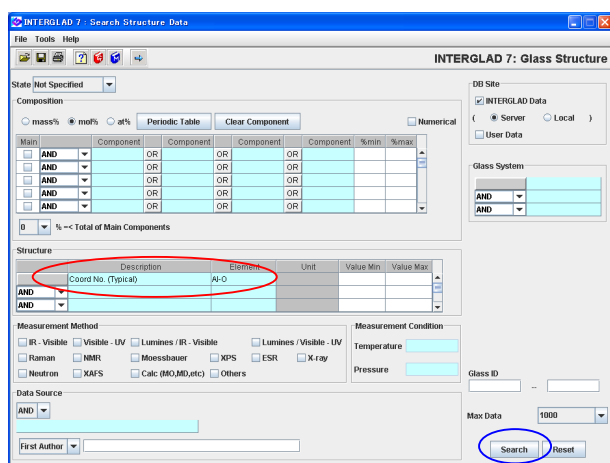


- All the searched glasses in this example contain alkali components. Relation between content of alkali oxides and fraction of non-bridging oxygen is checked in this XY Plot of content of $\text{Li}_2\text{O}+\text{Na}_2\text{O}+\text{K}_2\text{O}$ vs. $\text{NBO}/[\text{totalO}](\text{O})$. It is found that the NBO fraction increases proportionally with increasing the alkali content.

4.4 Investigation of correlation between structure and property — Coordination number of Al-O and properties

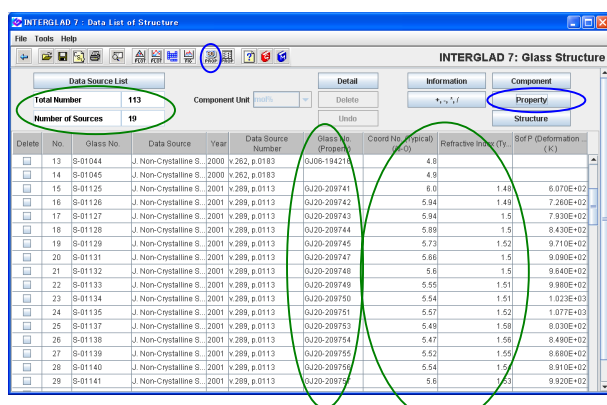
< Refer to E of Chapter 3, and 5 of Chapter 4 >

1) Specification of search conditions ([Search Structure Data] window) → Search



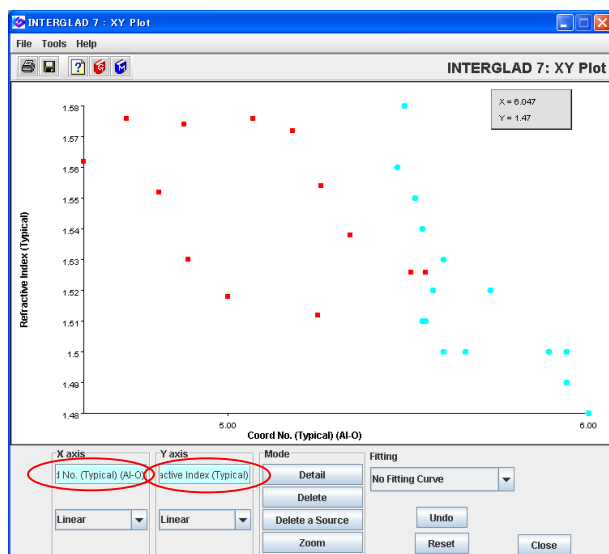
- Specify 'Coord No. (Typical)' for the Description of the Structure, and 'Al-O' for the Element. This means coordination number of O around Al.

2) Search result ([Data List of Structure] window)

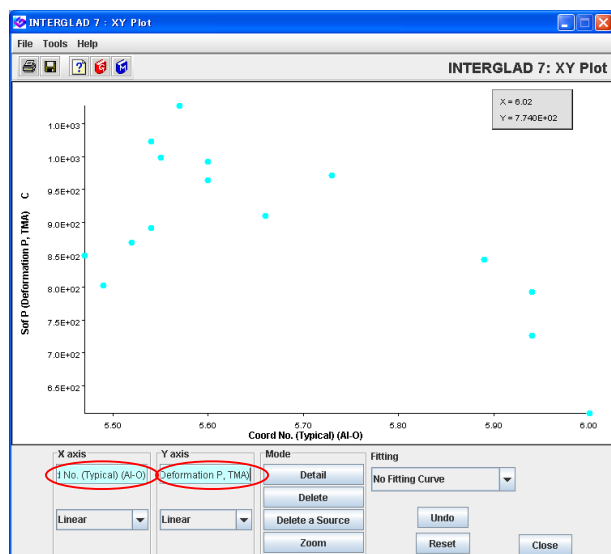


- 113 glasses of 19 data sources are listed.
- By clicking the [Search Property DB] icon, Glass Nos. of the corresponding glasses in the Property Database appear in the list.
- To check the corresponding property data, click the [Property] button, and select 'Refractive Index (Typical)' and 'Sof P (Deformation P, TMA)' in the [Select Property] dialog box opened. The data columns of Coord No. (Typical), Refractive Index (Typical) and Sof P (Deformation P, TMA) are dragged to the left for easy confirmation like the list of the figure.

3) Correlation between coordination number of Al-O and properties ([XY Plot] window)



- An XY Plot of Coord No. (Typical) (Al-O) vs. Refractive Index (Typical) is shown.
- The relation between the coordination number and the refractive index is not clear due to data scattering. It seems that the refractive index decreases with increasing the coordination number.

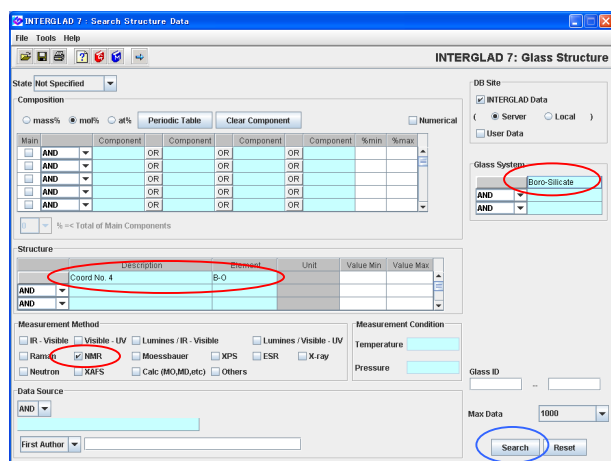


- This window shows an XY Plot of Coord No. (Typical) (Al-O) vs. Sof P. The tendency is not clear due to data scattering, although it seems that the curve has a peak around 5.6 of the coordination number.
- Under present, INTERGLAD has few glasses which have structure data and property data both.

4.5 Investigation of structure data analyzed by a specified method — 4-fold coordinated B atoms of boro-silicate glasses analyzed by NMR

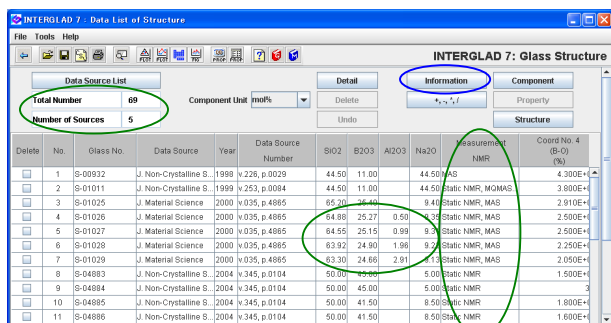
< Refer to E of Chapter 3, and 5 of Chapter 4 >

1) Specification of search conditions ([Search Structure Data] window) → Search



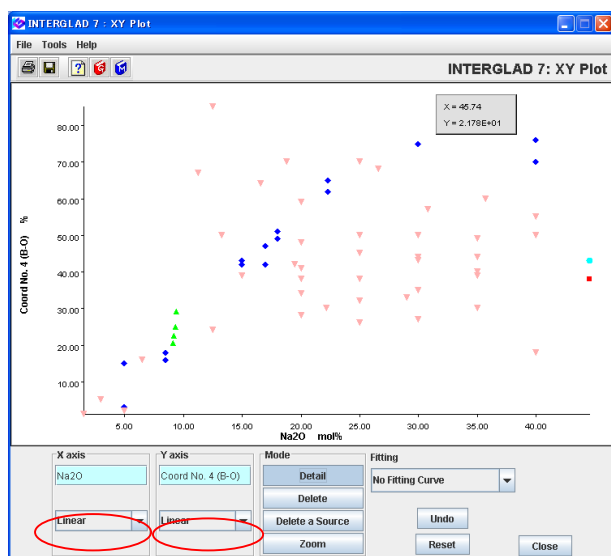
- This
- Select 'Boro-Silicate' for the Glass System, 'Coord No.4' for the Description of the Structure, and 'B-O' for the Element. 'Coord No.4 (B-O)' means 4-fold coordinated B atoms.
- Check in the checkbox of 'NMR' in the [Measurement Method] column.

2) Search result ([Data List of Structure] window)



- 69 glasses of 5 data sources are listed.
- Click the [Component] button to open the [Select Structure] dialog box, and select 'Select All'. It is found that all the glasses are those of $\text{SiO}_2\text{-B}_2\text{O}_3\text{-Na}_2\text{O}$ system. 4 glasses contain less than 3 mol% of Al_2O_3 .
- Click the [Information] button, and select 'Measurement' in the [Information Select] dialog box. The user can know that all the fractions of the 4-fold coordinated B atoms are data analyzed using NMR.

3) Utilization of search result ([XY Plot] window)



- This window shows an XY Plot of ‘Coord No.4 (B-O)’ vs. Na₂O content. The fraction of 4-fold coordinated B atoms has a large scattering in the range of over 10mol% Na₂O.