## **Examples of Use**

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### [Search and Analysis of Structure Data]

12. Investigation of correlation between composition and structure

- SiO<sub>2</sub> content and bridging oxygen fraction

13. Investigation of correlation between structure factors

 $-Q^2$  and non-bridging oxygen fraction of alkali-silicate glasses

### Notes

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



- 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 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<sub>2</sub>O or K<sub>2</sub>O, 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)
  - $\rightarrow$  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)



- 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)

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File To	ools H	elp													
4	<b>\$</b>	1 🔁 🖨 🖓	A K			1 2 1	?	6		INT	ERGLAD 7	Glas	s Prope	ərt	у
	•	Data Source Li	st				$\triangleleft$	Detail	lr	formation	n Comp	onent			^
	T	otal Number	248 Compone			mass%	- [	Delete		*, -, <sup>1</sup> , /	Pro	erty			
	N	umber of Sources	59	Proper	ty Unit	Common	-	Undo	Addi	livity Equa	tion Stru	cture			
Delete	No.	Glass No.	Da	ta Source	Year	Data So Numb	urce ler	AI2O3	Na2O	K20	Expansion Coeff (	y>			
	8	GC20-051404	Corning	Inc (US)		4602		14.00	0.89		5.400E	87			
	163	GI20-191886R	NGF's A	dditional N	2001	v.004, p.0009	9	10.26	4.00E		5.617E+	01			
	70	GP20-125149	US Pate	ent	1992	A5173456		13.33		2.01	5.934E+	01		П	
	86	GP20-125482	Europe	an Patent	1992	A0492577		13.33		2.01	5.934E+	01			
	136	GP20-154889	Japane	se Patent	1994	A040743		11.96		1.80	5.934E+	01			
	74	GP20-125157	US Pate	ent	1992	A5173456		11.96		0.74	6.040E+	01			
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🧽 INTERGLAI	D7 : Detail Dat	a of Property						X				
File Tools H	elp											
🗃 🖗 [	? 😺 😺		INTERGLAD7: Glass Property									
Glass No.		State	Prop	erties								
6020	-051404	Glass	ID	Specified	Value	Unit	Condition					
0020	-001404		0510	Density at RT	2520.0	kg/m3		1±				
Composition			0540	0540 Young's Modulus at RT 7.096E10 Pa								
Condition of I	Data	Glass System	1021	Expansion Coeff (0~300C)	54.0	10-7/K		1				
Т	arget	Alumino-Silicate	1113	T at 1E4 dPa.s (Working P)	1306.0	K		1				
<u> </u>		Phosphate	1116	T at 1E7.6(7.65) dPa.s (Sof P)	1033.0	к		-				
Components		Thoophate	1119	T at 1E13 dPa.s (Annealing P)	833.0	K		1				
1	mass%		1122	T at 1E14 dPa.s (Strain P)	792.0	к		1				
Si02	18.37 🔺	Filler / Crystal / Substrate	2018	Refract Index 589.3nm D	1.51			1				
AJ2O3	14.00	/ Dotto Chopp	5010	Water Durability Other	3.0							
Li20	0.20	7 Railo onape	5011	Water Durability ASTM	3.0			1_				
Na2O	0.89		6020	Acid Registance Other	4.0			-				
FeO	1.29		Autho	ors								
ZnO	4.17											
SnO	2.68 🗸	Sol-Gel Material										
Commercial	Glass		Data	Source								
commercial	oluoo		Cornir	ng Inc (US)								
Corn	ing 4602		4602.0									
		Change & Facebook	Mem	D								
Usaye		shape & reaulte										
Wavelength S	elector											
			Note									
			Heat Absorbing									
Thermal Treat	ment			Figure 🔻	Close							

• 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] wind	ow
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🤕 IN	TERGLAD 7 : Data Sour	ce List										
File	Tools Help											
	😂 🖓 📝 🔞 🚳			INTERGLAD 7: Data Source Lis								
	Data Source	Year	Data Source Number	Author	Merno	Jum of Data						
1	Phys. & Chem. Glasses	1997	Vol. 038 Page 0015	Montagne L., Palavit G.,		0						
2	J. Material Science	1997	Vol. 032 Page 5851	Donald I.W., Metcalfe B.L		70						
3	European Patent	1990	A0356746			58						
4	J. Non-Crystalline Solids	2001	Vol. 288 Page 0008	Karabulut M., Melnik E., S	Melting : in alumina cruc.	.11 =						
5	US Patent	2004	A6784128			10						
6	Japanese Patent	2007	A290886			10						
7	Data Book of Glasses C	1991	Vol. 001 Page 0120			5						
8	Glass Phys. & ChemUS	2004	Vol. 030 Page 0425	Batyaev I.M., Leonov A.V.	Melting : in alundum cru	1						
9	US Patent	1992	A5173456			61						
10	European Patent	2003	A1275622			10						
11	Glass Technology	1991	Vol. 032 Page 0166	Peng Y.B., Day D.E.		26						
12	Japanese Patent	1994	A107428			8						
13	J. Am. Ceram. Soc.	1981	Vol. 064 Page 0206	Abe Y., Kawashima K., S		2						
14	Japanese Patent	1981	A051574			10						
15	US Patent	2003	A0153450			10						
16	US Patent	2005	A0159291			8						
17	J. Non-Crystalline Solids	1997	Vol. 222 Page 0396	Brow R.K., Tallant D.R.		28						
18	Bull. Mater. Sci.	2003	Vol. 026 Page 0715	Shah K.V., Sudarsan V.,	Melting: in Pt crucible at 8	۸ /-						
			C	lose		$\bigcirc$						

- 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.

[Data Source List] window

### 2. Ternary plot analysis of property data

- Thermal expansion coefficient of SiO<sub>2</sub>-TiO<sub>2</sub>-Na<sub>2</sub>O glasses

Investigate relation between composition and thermal expansion coefficient on SiO<sub>2</sub>-TiO<sub>2</sub>-Na<sub>2</sub>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<sub>2</sub>, TiO<sub>2</sub> and Na<sub>2</sub>O.
- Select 'Expansion Coeff (Typical)' for the Specified of the Property.

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

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<b>(</b>	2	38 8	응 젊 등 🖷	and an		1 🖸 🚺		IN	TERGLAD 7: G	lass Property
		Data Source Li	ist			Detail	In	formati	on Compone	ent
	To	tal Number	200 Comp	onent Unit	mass% 💌	Delete		+, -, 1, 7	Propert	y
	N	mber of Sources	37 Pro	operty Unit	Common 👻	Undo	Addit	ivity Equ	ation Structur	e
Delete	No.	Glass No.	Data Source	Year	Data Source Number	SIO2	Na20	TIO2	Expansion Coeff (Ty (10-7/K)	
	1	GB02-006032	Handbook of Glas	s 1986	v.001, p.0163	67.08	15.21	17.71	8.400E+01	-
	2	OB02-006033	Handbook of Glas	s 1986	v.001, p.0163	51.85	15.56	32.58	1.100E+02	-
	3	GB02-006034	Handbook of Glas	s 1986	v.001, p.0163	49.04	20.56	30.40	1.120E+02	-
	4	GB02-006035	Handbook of Glas	s 1986	v.001, p.0163	35.56	20.57	43.87	1.080E+02	
	5	GB02-006036	Handbook of Glas	s 1986	v.001, p.0163	42.29	21.44	36.27	1.160E+02	
	6	GB02-006037	Handbook of Glas	s 1986	v.001, p.0163	69.61	23.39	6.99	1.100E+02	
	7	GB02-006038	Handbook of Glas	s 1986	v.001, p.0163	50.68	22.51	26.81	1.070E+02	
	8	GB02-006039	Handbook of Glas	s 1986	v.001, p.0163	30.71	22.63	46.66	1.150E+02	
	9	GB02-006040	Handbook of Glas	s 1986	v.001, p.0163	58.00	25.69	16.31	1.180E+02	
	10	GB02-006041	Handbook of Glas	s 1986	v.001, p.0163	42.61	26.03	31.36	1.160E+02	
	11	GB02-006042	Handbook of Glas	s 1986	v.001, p.0163	53.26	26.93	19.80	1.270E+02	

### 3) Ternary plot



• 200 glasses are searched.

- Open the [Ternary Plot] window by clicking the [Ternary Plot] icon. Select SiO<sub>2</sub>, TiO<sub>2</sub> and Na<sub>2</sub>O 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 SiO<sub>2</sub> 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 ≤ 100×10<sup>-7</sup>/K, and the ternary diagram with SiO<sub>2</sub> (100%), Na<sub>2</sub>O (50%), TiO<sub>2</sub> (50%) is shown by using the [Zoom] button.

### 3. 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  $\rightarrow$  Search



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

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		Data Source L	ist			Detail	Infor	mation	Component	<b>^</b>
	Tot	al Number	3302 Compo	ient Uni	t mot% 💌	Delete	+,	557	Property	
	Nu	mber of Sources	2281 Prop	erty Uni	t Common 👻	Undo	Additivit	y Equation	Structure	
Delete	No.	Glass No.	Data Source	Year	Data Source Number	Refract li	ndex 587.6	Abbe Value (nd-	1)/(	
	1	GJ05-008626	Glastech. Ber.	1987	v.060, p.0234		1.502	6.560E	+01	-
	2	GJ05-008627	Glastech. Ber.	1987	v.060, p.0234		1.502	6.620E	+01	
	3	GJ05-008628	Glastech. Ber.	1987	v.060, p.0234		1.503	6.6528	+01	
	4	0J05-008629	Glastech. Ber.	1987	v.060, p.0234		1.502	6.665E	+01	_
	5	GJ05-008630	Glastech. Ber.	1987	v.060, p.0234		1.503	6.670E	+01	
	6	0J05-008631	Glastech. Ber.	1987	v.060, p.0234		1.503	6.659E	+01	
	7	GJ05-008632	Glastech. Ber.	1987	v.060, p.0234		1.504	6.685E	+01	
	8	OJ05-008633	Glastech. Ber.	1987	v.060, p.0234		1.504	6.7228	+01	
	9	GJ05-008634	Glastech. Ber.	1987	v.060, p.0234		1.503	6.723E	+01	
	10	GJ01-014872	J. Ceram. Soc. Japa	n 1985	v.093, p.0498		1.462	6.750E	+01	
	11	GB03-017329	Handbook of Glass.	. 1987	v.00C, p.0910		1.611	5.350E	+01	
	12	OB03-017330	Handbook of Glass.	. 1987	v.00C, p.0910		1.621	5.320E	+01	
	13	GB03-017331	Handbook of Glass.	. 1987	v.00C, p.0910		1.637	5.230E	+01	
	14	OB03-017332	Handbook of Glass.	. 1987	v.00C, p.0910		1.644	6.190E	+01	
	15	GB03-017333	Handbook of Glass.	. 1987	v.00C, p.0910		1.663	5.030E	+01	
	16	GB03-017334	Handbook of Glass.	. 1987	v.00C, p.0910		1.661	5.100E	+01	

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



- 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.

• 3302 glasses are listed.

- 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.

## 4. 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
  - $\rightarrow$  Search



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

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		Data Source	List			Detail	Inform	nation	Component	
	$\triangleleft$	Total Number	868 Compo	nent Unit	mol%i 💌	Delete	+,.	s. 57	Property	
		Number of Source	s 163 Prop	erty Unit	Common 💌	Undo	Additivity	/Equation	Structure	
Delete	No.	Glass No.	Data Source	Year	Data Sour Number	ce Visco	sity 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					8
	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					
	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					
	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	OB05-010248	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					
	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+07			<b>v</b>

3) Data interpolation or extrapolation

- 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.

- 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.

• 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

🐼 Select Data Interpolation Condition 🛛 🛛 🔀
Specify interpolation method.
Viscosity
Interpolation Condition
🖌 Avoid to interpolate beyond Tg : Rough Tg 🔤 C
Avoid to interpolate too away : Limit = ± 200 💌 deg
Interpolation Equation —
Inear interpolation
n-th order polynomial interpolation
Variable
y (property): 🔾 y 🔾 1/y 🖲 log y
x (temperature or viscosity): 🔾 x 💿 1/x 🔷 log x
🕢 use absolute temperature (K)
OK CANCEL

🥝 INTE	RGL/	AD 7 : Data List o	of Property					
File To	ols	nalp	0					
4		388			🧝 🖬 [	) 😺 😺	INTERG	LAD 7: Glass Property
		Data Source	List			Detail	Information	Component
		Total Number	868 Co	mponent Uni	it mol% 💌	Delete	+, -, *, /	Property
		Number of Source	s 163	Property Uni	t Common 💌	Undo	Additivity Equation	Structure
Delete	No	. Glass No.	Data Sourc	e Year	Data Source Number	Viscosit (dF	yat 700C 'a.s.)	
	1	GJ02-000026	Glastech. Ber.	1983	v.056, p.0125			
	2	GB04-004679	Handbook of Gla	ss 1986	v.001, p.0299	1		=
	3	GB04-004680	Handbook of Gl	ass 1986	v.001, p.0299		2.692E+01	
	4	GB04-004681	Handbook of Gl	ass 1986	v.001, p.0299		1.0E+01	
	5	GB04-004682	Handbook of Gla	iss 1986	v.001, p.0299			
	6	GB04-004683	Handbook of Gl	ss 1986	v.001, p.0299		1.167E+03	
	7	GB04-004684	Handbook of Gl	ass 1986	v.001, p.0299			
	8	GJ05-005435	J. Am. Ceram. S	oc. 1980	v.063, p.0126		2.0E+10	
	9	GJ05-010069	J. Am. Ceram. S	oc. 1974	v.057, p.0109	$\rightarrow$	7.973E+07	
	10	GJ05-010070	J. Am. Ceram. S	oc. 1974	v.057, p.0109		7.311E+09	
	11	GB05-010245	Handbook of Gla	ass 1986	v.001, p.0243			
	12	GB05-010246	Handbook of Gl	ass 1986	v.001, p.0243			
	13	GB05-010247	Handbook of Gla	ss 1986	v.001, p.0243			
	14	GB05-010248	Handbook of Gl	ass 1986	v.001, p.0243			
	15	GB05-010249	Handbook of Gl	ass 1986	v.001, p.0244		1.622E+03	
	16	GB05-010250	Handbook of Gl	ass 1986	v.001, p.0244		1.005E+03	
	17	GB05-010253	Handbook of Gl	ass 1986	v.001, p.0244		3.162E+03	
	18	GB05-010254	Handbook of Gl	ass 1986	v.001, p.0244			
	19	GB05-010255	Handbook of Gl	ass 1986	v.001, p.0244		1.514E+04	
	20	GB05-010256	Handbook of Gl	ass 1986	v.001, p.0244			
	21	GB05-010257	Handbook of Gl	ass 1986	v.001, p.0244		2.188E+05	
	22	GB05-010259	Handbook of Gl	ass 1986	v.001, p.0244		2.754E+06	
	23	GB05-010260	Handbook of Gla	iss 1986	v.001, p.0244		2.692E+07	-

temperature (K)] checkbox. Then click the [OK] button.

- 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  $700 \pm 200$ °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)

### 5. Search of commercial glasses – High strength glass fiber for FRP

Investigate commercial glasses of high strength glass fiber for FRP.

 $<\!{\rm Refer}$  to B of Chapter 3, and 2 of Chapter  $4\!>$ 

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

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- 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)

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		Data Source Li	st				Detail	Inform	ation	Component	
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	N	umber of Sources	18	Propert	y Unit	Common 💌	Undo	Additivity E	Equation	Structure	
Delete	No.	Glass No.	Da	ta Source	Year	Data Source Number	Young's	Modulus at.	Tensile Stre (MPa)	ength	
	10	GC06-052346	Nitto Bo	iseki (J)		NITTOBOT-GLASS	3		4.65	5E+03	
	4	GC06-052225	Owens	Corning (US)	1989	9 Glass		8.550E+01	4.58	35E+03	
	3	GC03-052224	Owens	Coming (US)	1989	E-Glass		7.230E+01	3.44	I5E+03	
	6	GC03-052249	Asahi F	iber Glass (J)		E-Glass		7.252E+01	3.43	0E+03	
	7	GC03-052250	Asahi F	iber Glass (J)		ECR-Glass		7.223E+01	3.43	0E+03	
	9	GC03-052344	Nitto Bo	iseki (J)		NITTOBOE-GLAS	3		3.43	30E+03	
	5	GC03-052228	America	an Biomateri	1989	C-Glass		6.890E+01	3.3*	I0E+03	
	12	GC02-052349	Nitto Bo	iseki (J)		NITTOBOC-GLAS	8		3.08	87E+03	
	11	GC05-052348	Nitto Bo	iseki (J)		NITTOBOD-GLAS	s		2.25	54E+03	
	8	GC05-052262	Central	Glass (J)		E-GLASSFIBER		7.252E+01	1.96	0E+03	
	13	GC03-052753	PPG Inc	i. (US)		FIBER GLASS			1.70	00E+03	
	2	GC03-052074	Nippon	Sheet Glas		E-Glass		7.350E+01	1.43	0E+03	
	14	GC03-071205	Nippon	Electric Gla	1989	EF		7.252E+01	1.45	/0E+03	
	1	GC03-051554	Corning	Inc (US)		E-Glass		7.400E+01			
	15	GC05-071206	Nippon	Electric Gla	1989	D-40					
	16	GC03-144895	Saint-G	obain (FR)	1983	02418					
	17	GC06-144896	Saint-G	obain (FR)	1983	0320180					
	18	GC06-144897	Saint-G	obain (FR)	1985	02509					



- 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

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		AND	-		OR	OR	OR			-	Sol-Gel				
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		Number o	f Sources 9	Prope	rty Unit Common 👻	Uni	to	Additiv	ity Equation	Structure	
Delete	No.	Glass No.	Data Source	Year	Data Source Number	SiO2	AJ2O3	MgO	Density at K1 (gicm3)	Young's Modulus (GPa)	Tensile Strengt (MPa)
	1	GB06-001791	Handbook of Glass	1986	v.001, p.0093	65.00	25.00	10.00	2.5		
	2	XJ03-032345	Glass Phys. & Che	1980	v.006, p.0444	65.00	25.00	10.00	2.5		
	3	GC08-051555	Corning Inc (US)		S-Glass	65.00	25.00	10.00			
	4	GC06-052225	Owens Coming (US)	1989	S-Glass	65.00	25.00	10.00	2.46	8.550E+01	4.585E+03
	5	GB06-164715	Fundamentals Inor	1994	v.001, p.0003	65.00	25.00	10.00			
	6	GJ06-172039	J. Non-Crystalline S	1997	v.209, p.0069	65.00	25.00	10.00			
	7	GB06-174772	Data Book of Glass	1991	v.001, p.0134	65.00	25.00	10.00	2.49	8.624E+01	4.606E+03
	8	GP06-205434	Japanese Patent	2000	A233942	65.00	25.00	10.00	<hr/>		
	9	GP06-300017	European Patent	2010	A2221335	65.00	25.00	10.00			

### 4) Investigation of data around S-Glass



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Delete	No.	Glass No.	Data Sour	ce	Year	Data	Source	8102	AI203	MgO	Young's Modulus at	Tensile Strength	-
		GJ06-073521	Glass Phys. & ChemU	SSR 1	982	v.008, p.00	026	64.98	26.58	8.44	9.200E+01	( 11 1)	-
	21	GJ06-073520	Glass Phys. & Chem.+O	san I	1002	v.999, p.04	26	66.69	24.00	9.01	9.100E+01		
	30	GB06-174772	Data Book of Glasses C	omposition (J) 1	1991	v.001, p.01	34	65.00	25.00	10.00	8.624E+01	4.606E+03	
	23	0806-089932	Glass Hand Book (J)	1	975	v.001, p.03	219	64.36	24.82	10.31	8.575E+01		П
	18	GC08-052225	Owens Coming (US)	1	1989	S-Glass		65.00	25.00	10.00	8.550E+01	4.585E+03	
	1	GB06-001787	Handbook of Glass Prop	perties 1	986	v.001, p.00	93	63.00	25.00	12.00			
	2	0806-001790	Handbook of Glass Prop	perties 1	986	v.001, p.00	93	66.30	23.30	10.40			
	3	GB06-001791	Handbook of Glass Prop	perties 1	986	v.001, p.00	93	65.00	25.00	10.00			
	4	0806-001792	Handbook of Glass Prop	perties 1	986	v.001, p.00	93	65.50	25.00	9.50			÷

- 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.
- 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.

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	Data Source :	Glass	Phys. & Cl	1emUSSF	ι	Number of Data :	5							
	Data Source Number	r: Vol. O	08 Page O	D26 (1982)		Component Unit	mass% 💌							
	Aslanova M.S., Dorzhiev D.B., Sapozhkova L.A., Author : Gorbachev V.V., Bystrikov A.S., Petrakov V.N., Property Unit SI 🔽													
	Memo : Detail													
	Glass No.	SIO2	AI2O3	MgO	Vickers Hardness ( (Pa)	Density at RT (kg/m3)	Young's Modulus at (Pa)	R						
1	GJ06-073518	69.50	16.92	13.58		2.510E+03	9.300E+10							
2	GJ06-073519	68.11	19.90	11.99	6.174E+09	2.492E+03	9.100E+10	٦						
3	GJ06-073520	66.09	24.30	9.61	5.880E+09	2.485E+03	9.100E+10	٦						
4	GJ06-073521	64.98	26.58	8.44	6.174E+09	2.495E+03	9.200E+10							
5	GJ06-073522	63.58	29.56	6.85	6.370E+09	2.500E+03	9.400E+10	٦						
	4			II				Þ						
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[Glasses from a Data Source] window

• 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.

# 6. Property prediction of glasses with a specified composition by additivity equations Boro-silicate glasses

## Predict density, thermal expansion coefficient and refractive index of boro-silicate glasses with $SiO_2$ 40%, $B_2O_3$ 30%, $Al_2O_3$ 10%, $Na_2O$ 10% and BaO 10% (mass%).

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

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

2) Prediction of thermal expansion coefficient

- 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/cm<sup>3</sup> appears in the [Predictive Value] column.
- 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]



### 3) Prediction of thermal conductivity





### 4) Prediction of refractive index

menu.

• Clicking the [Calculate] button shows the predictive value 6.862 × 10<sup>-6</sup>/K in the [Predictive Value] column.

- 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<sup>-1</sup> 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  $8.349 \times 10^{-1}$  W/(mK) (0°C) and  $9.256 \times 10^{-1}$  W/(mK) (0°C) are obtained respectively. The user can compare the results by the difference of additivity equations.
- 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>

## 7. Obtaining an additivity equation (multiple regression 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)  $\rightarrow$  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)

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Delete	No.	Glass No.	Da	a Source	Year	Data Source Number	Density at RT (g/cm3)	Density at RT (Predictive Value)	Density at R (Residual)	٦.
	1	GB02-000500	Handbo	ok of Glass	1986	v.001, p.0065	2.74			-
	2	GB02-000501	Handbo	ok of Glass	1986	v.001, p.0065	2.867			3
	3	GB02-000502	Handbo	ok of Glass	1986	v.001, p.0065	2.99			
	4	GB02-000503	Handbo	ok of Glass	1986	v.001, p.0065	3.115			
	5	GB02-000504	Handbo	ok of Glass	1986	v.001, p.0065	2.405			
	6	GB02-000505	Handbo	ok of Glass	1986	v.001, p.0065	2.51			
	7	GB02-000506	Handbo	ok of Glass	1986	v.001, p.0065	2.636			
	8	GB02-000507	Handbo	ok of Glass	1986	v.001, p.0065	2.885			
	9	GB02-000508	Handbo	ok of Glass	1986	v.001, p.0065	2.439			
	10	GB02-000509	Handbo	ok of Glass	1986	v.001, p.0065	2.55			-

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	🖌 Min. num. of gla	sses = 1 %	of total retrived glasses										
	🗹 Min. num. of gla	sses = 2 gla	isses to one component										
	Select All C	omponent Clea	r All Component										
	Component	Number of Glasses	s Max. Content %										
r	SiO2	32	5 85.000										
r	B2O3	12	3 50.000										
r	AI2O3	15	3 22.500										
2	MgO	1	1 30.000										
V	CaO	9	1 30.000										
V	BaO	4	9 30.000										
1	Li2O	2	3 35.000										
1	Na2O	12	0 40.000										
1	K20	9	7 35.000										
~	MnO		5 45.000										
	FeO		1 0.540										
~	CuO		5 3.140										
~	ZnO	32	2 70.000										
~	Sr0	1	8 30.000										
	CdO		1 40.000										
r	PbO	1	7 40.000										
	SnO		0 0.000										
	Cr203		0 0.000										

•	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.



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	1	GB02-000500	ndbook	of Glass	1986	v.001, p.0065	65.00						15.00		
	2	GB02-000501	ndbook	of Glass	1986	v.001, p.0065	60.00						15.00	E	
	3	GB02-000502	ndbook	of Glass	1986	v.001, p.0065	55.00						15.00		
	4	GB02-000503	ndbook	of Glass	1986	v.001, p.0065	50.00						15.00	1	
	5	GB02-000504	ndbook	of Glass	1986	v.001, p.0065	75.00						20.00	1	
	6	GB02-000505	ndbook	of Glass	1986	v.001, p.0065	70.00						20.00	1	
	7	GB02-000506	ndbook	of Glass	1986	v.001, p.0065	65.00						20.00		
	8	GB02-000507	ndbook	of Glass	1986	v.001, p.0065	55.00						20.00	1	
	9	GB02-000508	ndbook	of Glass	1986	v.001, p.0065	70.00						25.00	1	
	10	GB02-000509	ndbook	of Glass	1986	v.001, p.0065	65.00						25.00		¥

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

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

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R	CaO				0.05536	91	Figure				
V	BaO				0.28831	49	Figure				
2	Li20				-0.18686	23	Figure	-			
V	Na2O				-0.39027	120	Figure				
V	к20				-0.23398	97	Figure				
Ľ	MnO				0.10783	5	Figure				
V	CuO				-0.09197	5	Figure				
r	ZnO				0.41101	322	Figure				
V	SrO				0.09525	18	Figure				
2	PbO				0.25174	17	Figure				
	Fe203				-0.15693	10	Figure				
	As203				0.06022	45	Figure				
~	Y203				0.31102	23	Figure	Ŧ			

QUEST	юм 🛛
?	All components of some glasses have the same values. Are the first glass data used for analysis, and are other glass data not used? The Delete checkboxes in glass list attach checks to the glass data not used.
	OK Cancel

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variable	ey: ⊛y ⊖ 1åj	r 🔾 log y	Exclude	2.003 + Com	ponenc cerms and	iei (d= 0.0 +		
					Component	Number	Component	
Select	Component	Conficient	Std. Error	tValue	vs Property		vs Property Correlation	
					Correlation	of Data	Plot	
~	Si02	2.28304E00	0.019	121.603	-0.38737	307	Figure	
~	B2O3	2.06361E00	0.065	31.750	0.19047	107	Figure	
V	AI203	2.49130E00	0.106	23.404	0.20420	143	Figure	
×.	MgO	3.48167E00	0.141	24.687	-0.03903	11	Figure	
V	CaO	3.50233E00	0.091	38.598	0.05536	82	Figure	
~	BaO	6.68162E00	0.081	82.132	0.28831	49	Figure	
~	Li20	2.34709E00	0.072	32.684	-0.18686	23	Figure	
2	Na2O	2.86601E00	0.069	41.367	+0.39027	119	Figure	
r	K20	2.48826E00	0.064	38.998	-0.23398	97	Figure	
~	MnO	4.73646E00	0.096	49.162	0.10783	5	Figure	41
V	CuO	4.02683E00	1.505	2.675	-0.09197	5	Figure	41
2	Zn0	4.79427E00	0.030	158.267	0.41101	304	Figure	
V	Sr0	5.24511E00	0.126	41.645	0.09525	18	Figure	41
V	Pb0	8.22720E00	0.158	52.041	0.25174	17	Figure	
~	Fe2O3	-1.63275E02	95.812	-1.704	-0.15693	10	Figure	
r	As203	2.60116E00	6.699	0.368	0.06022	45	Figure	
~	Y203	8.29549E00	0.138	60.311	0.31102	23	Figure	

• 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  $\geq 0.8$  as the  $R^2$  is recommended.

#### 5) t value check $\rightarrow$ 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.</li>
- In this example, |t| of Fe<sub>2</sub>O<sub>3</sub>, As<sub>2</sub>O<sub>3</sub> and Sb<sub>2</sub>O<sub>3</sub> are <2. First, delete ✓ in the checkboxes of As<sub>2</sub>O and Sb<sub>2</sub>O<sub>3</sub> with |t|<1, and recalculate. Second, delete ✓ in the checkbox of Fe<sub>2</sub>O<sub>3</sub> with |t|<2, and recalculate. By these procedures the component terms with |t|<2 are removed from the multiple regression equation.</li>
- Verification of the multiple regression analysis is performed again. R<sup>2</sup> 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:

Density at RT (g/cm<sup>3</sup>) =  $2.273 \times (SiO_2) + 2.051 \times (B_2O_3) + 2.503 \times (Al_2O_3) + \dots$ 

 $(SiO_2), (B_2O_3), \dots : mole ratio of each component (20 components except others)$ 

• 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.

### 8. Property prediction by multiple regression analysis – Density of zinc-silicate glasses Predict density at RT of a glass with SiO<sub>2</sub> 60%, Li<sub>2</sub>O 20% and ZnO 20% (mol%).

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

The multiple regression equation obtained in 7. is used because of the same zinc-silicate glass system.

1) Regression analysis result  $\rightarrow$  Transit to the [Property Prediction] window

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				$\cup$			Detail							1
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	N	umber of Sources	110	Proper	ty Unit	Common 💌			Compor	ient	Analy	ze		
Delete	No.	Glass No.	Da	ta Source	Year	Data Source Number	SiO2	B2O3	AI203	MgO	CaO	BaO	Li2O	
	1	GB02-000500	Handbo	iok of Glass	1986	v.001, p.0065	65.00						15.0	-
	2	GB02-000501	Handbo	ok of Glass	1986	Y.001, p.0065	60.00						15.0	
	3	GB02-000502	Handbo	iok of Glass	1986	v.001, p.0065	55.00						15.0	
	4	GB02-000503	Handbo	iok of Glass	1986	v.001, p.0065	50.00						15.0	
	5	GB02-000504	Handbo	iok of Glass	1986	v.001, p.0065	75.00						20.0	
	6	GB02-000505	Handbo	iok of Glass	1986	v.001, p.0065	70.00						20.0	
	7	GB02-000506	Handbo	iok of Glass	1986	v.001, p.0065	65.00						20.0	H
	8	GB02-000507	Handbo	iok of Glass	1986	v.001, p.0065	55.00						20.0	
	9	GB02-000508	Handbo	iok of Glass	1986	v.001, p.0065	70.00						25.0	
	10	GB02-000509	Handbo	iok of Glass	1986	v.001, p.0065	65.00						25.0	
	11	GB02-000510	Handbo	iok of Glass	1986	v.001, p.0065	50.00						31.2	
	12	GB02-000511	Handbo	iok of Glass	1986	v.001, p.0065	65.00						30.0	-



- 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 7. 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.

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8 🔂 🙎	) 😺 😺				INTER	RGLAD7: Pro	perty Prediction
Regression Ed	quation						
		Coefficient				Content (mol%)	
Component	Density at RT				Initial	New	
SiO2	2.273E00					60.000	
B203	2.051E00					0.000	
AI2O3	2.503E00					0.000	Glass-Forming Region
MgO	3.487E00					0.000	
CaO	3.512E00					0.000	
BaO	6.644E00					0.000	
Li20	2.366E00					20.000	
Na20	2.868E00					0.000	
K20	2.502E00					0.000	$\frown$
MnO	4.746E00					0.000	Calculate
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Property				-	-		
	Specified		Unit	Predictive V	alue	$\sim$	
🔶 Density	atRT		g/cm3		2.798		
•					_		

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/cm<sup>3</sup>.

## 9. Composition optimization by multiple regression analysis - Zinc-silicate glass with a specified density

Obtain a composition of zinc-silicate glass with 2.6 g/cm<sup>3</sup> of density at RT. The components of the glass are SiO<sub>2</sub>, B<sub>2</sub>O<sub>3</sub>, Na<sub>2</sub>O, and ZnO.

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

The multiple regression equation obtained in 7. is used because of the same zinc-silicate glass system.

1) Regression analysis result  $\rightarrow$  Transit to the [Composition Optimization] window



### 2) Composition optimization



- 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 7. 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/cm<sup>3</sup> of density as a model.
- By clicking the [COMP] icon, the [Composition Optimization] window opens.
- 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 SiO<sub>2</sub>, B<sub>2</sub>O<sub>3</sub>, Na<sub>2</sub>O and ZnO referring the initial (model) values. In this example enter the close integral numbers of the initial values for SiO<sub>2</sub>, B<sub>2</sub>O<sub>3</sub> and ZnO, and 10 for B<sub>2</sub>O<sub>3</sub>. 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/cm<sup>3</sup> in case of the following composition. The composition: SiO<sub>2</sub> 66.3%, B<sub>2</sub>O<sub>3</sub> 9.0%, Na<sub>2</sub>O 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 SiO<sub>2</sub>-Na<sub>2</sub>O-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.

### 10. Property prediction by a cubic multiple regression equation — Refraction index of boro-silicate glasses

Predict refraction index of glasses of SiO<sub>2</sub>-B<sub>2</sub>O<sub>3</sub>-R<sub>2</sub>O-RO system with the following composition. SiO<sub>2</sub> 65%, B<sub>2</sub>O<sub>3</sub> 10%, MgO 5%, CaO 4%, Na<sub>2</sub>O 7%, K2O 5%, Al<sub>2</sub>O<sub>3</sub> 4% (mass%).

 ${<}\mathrm{Refer}$  to D.2 of Chapter 3, 4.2-4.6 of Chapter 4 ${>}$ 

1) Specification of search conditions ([Search for Regression Analysis] window)  $\rightarrow$  Search

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×	AND	-	MgO	OR	CaO	OR		0R		0			
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 $\bullet$  Specify the following condition of composition.

 $SiO_2 + B_2O_3 + (Na_2O \text{ or } K_2O \ge 0)$ 

+ (MgO or  $CaO \ge 0$ )  $\ge 95$  mass%.

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

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

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	1	GJ05-008626	Glastech	Ber.	1987	v.060, p.023	73.	3 16.9	2		10.04			
	2	GJ05-008627	Glastech	Ber.	1987	v.060, p.023	72.	5 16.8	3		8.99	1.52		
	3	GJ05-008628	Glastech	Ber.	1987	v.060, p.023	71.3	1 16.6	6		6.92	4.51		1
	4	GJ05-008629	Glastech	Ber.	1987	v.060, p.023	71.	4 16.5	в		5.90	5.98		1
	5	GJ05-008630	Glastech	Ber.	1987	v.060, p.023	71.	7 18.4	9		4.89	7.44	1.50	2
	6	GJ05-008631	Glastech	Ber.	1987	v.060, p.023	70.	1 16.4	1		3.89	8.88		1
	7	GJ05-008632	Glastech	Ber.	1987	v.060, p.023	70.	6 16.3	3		2.91	10.31		1
	8	GJ05-008633	Glastech	Ber.	1987	v.060, p.023	69.	5 16.1	6		0.96	13.12		1
	9	GJ05-008634	Glastech	Ber.	1987	v.060, p.023	69.	1 16.0	в			14.51		1
	10	GB05-010781	Handboo	k of Glass	1986	v.001, p.054	8 84.1	9 15.3	1					1
	11	GB05-010782	Handboo	k of Glass	1986	v.001, p.054	8 83.0	1 16.1	9					1
	12	GB05-010783	Handboo	k of Glass	1986	v.001, p.054	3 77.5	4 22.4	6					1
	13	GB05-010784	Handboo	k of Glass	1986	v.001, p.054	64.3	1 35.2	в					1
	14	GB05-010785	Handboo	k of Glass	1986	v.001, p.054	63.3	2 36.6	в					1
	15	GB05-010786	Handboo	k of Glass	1986	v.001, p.054	3 4.9	9 95.0	1					1
	16	GB05-010787	Handboo	k of Glass	1986	v.001, p.054	84.1	9 15.3	1					
	17	GB05-010796	Handboo	k of Glass	1986	v.001, p.054	9 57.1	5 42.8	3					1
	18	GB05-010797	Handboo	k of Glass	1986	v.001, p.054	9 51.3	6 48.2	2					1
	19	GB05-010798	Handboo	k of Glass	1986	v.001, p.054	9 44.	2 55.2	6					
	20	GB05-010799	Handboo	k of Glass	1986	v.001, p.054	8 40.0	1 59.9	в					Н
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	Min. num. of gla	sses = 2	glas	ses to one compo	nent
Ľ					
	Select All Co	omponent	Clear	All Component	
	Component	Number of	Glasses	Max. Content %	
~	SiO2		740	97.440	
~	B2O3		740	98.080	
r	MgO		27	5.500	
r	CaO		84	16.000	
r	Na2O		532	39.910	
r	K20		221	42.940	
r	AI2O3		109	5.000	
r	BaO		15	3.000	
r	Li2O		16	4.960	
	MnO		1	0.004	
	FeO		2	0.085	
	Ce0		4	0.370	
	NIO		4	0.370	
V	ZnO		12	3.000	
	PbO		2	0.420	
V	Fe2O3		41	0.660	
V	As203		28	1.700	
V	Sb2O3		10	1.200	
	BACK	Nevt	OK	Cancel	

QUESTION
Selection of Explanatory Variables in Multiple Regression Analysis: Component Terms: 10 Component Terms: 0 Component Terms: 0 OK Cancel

- 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.

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	8102	1.47356E00	0.002	910.895	-0.19661	548	Figure	
	8203	1.46609E00	0.003	512.909	-0.26647	548	Figure	- 1
<b>V</b>	MgO	1.44104E00	0.113	12.779	0.14223	26	Figure	- 1
	CaO	1.82462E00	0.027	67.989	0.27276	81	Figure	- 1
<b>V</b>	Na2O	1.67562E00	0.006	290.579	0.57557	385	Figure	- 1
	K20	1.62266E00	0.005	307.179	0.17377	204	Figure	- 1
<b>v</b>	AI203	1.36068E00	0.065	20.820	-0.18826	96	Figure	- 1
	BaO	2.00095E00	0.138	14.451	0.02916	15	Figure	_ =
	LI20	2.11308EUU	0.136	15.559	-0.01464	14	Figure	- 1
	ZnO	1.48695E00	0.242	6.143	0.01392	11	Figure	- 1
	Fe2O3	1.56359E00	0.867	1.803	0.13034	38	Figure	
	AS2U3	1.2/896E00	0.339	3.770	-0.01974	25	Figure	-
	Sb203	9.58643E-01	0.651	1.473	0.04016	10	Figure	
	Nd2O3	1./1887E00	0.066	26.083	0.12850	14	Figure	-
	803	-7.89066E-01	1.942	-0.406	0.08736	10	Figure	
	H20	-2./3134E01	18.213	-1.500	-0.32268	13	Figure	
	R203	4.50009E00	1.609	2.796	0.02324	17	Figure	-

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







4) Regression analysis by a cubic equation

QUESTION
Selection of Explanatory Variables in Multiple Regression Analysis: Component Terms: 19 Component Terms: 15 Component Terms: 15 Component Terms: 1 OK Cancel

• 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.

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Select	Component	Coefficient	Std. Error	tValue	Component vs Property Correlation	Number of Data	Component vs Property Correlation Plot	
v.	Si02	1.45942E00	0.002	772.204	-0.21997	546	Figure	<u>_</u>
2	B2O3	1.45517E00	0.003	512.270	-0.24280	546	Figure	
×	MgO	1.56346E00	0.071	21.891	0.15950	26	Figure	
×	CaO	1.68703E00	0.322	5.244	0.31492	81	Figure	
	Na2O	1.11817E00	0.026	43.805	0.52650	383	Figure	-
×	K20	1.33035E00	0.02	53.938	0.20000	203	Figure	
	AI203	6.10373E00	2.43	2.603	-0.20908	95	Figure	
*	BaO	1.89497E00	0.078	25.843	0.03445	15	Figure	_
2	Li20	2.34043E00	0.070	33.634	-0.03637	13	Figure	
	ZnO	1.62611E00	0.12	13.047	0.00992	11	Figure	
K	Fe203	2.44618E00	0.47	5.160	0.14379	38	Figure	
×	As203	1.02791E00	0.180	5.706	-0.02981	25	Figure	
×	Sb203	1.72576E00	0.347	4.976	0.04850	10	Figure	
M	Nd203	1.82067E00	0.039	46.301	0.15746	14	Figure	
×	803	1.06650E00	1.037	1.028	0.10674	10	Figure	
M	H20	3.45907E01	10.790	3.206	-0.28171	13	Figure	
*	R203	3.68107E-01	0.811	0.45	0.02703	17	Figure	-





- Execute the regression analysis in the [Execution of Regression Analysis] window, and open the [Verification of Regression Analysis] window. R<sup>2</sup> 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).</li>
- 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.
  - 1) Exclude '2&3' component terms under |t| = '1.0.'
  - 2) Exclude '2&3' component terms under |t| = '2.0.'
  - 3) Exclude 'all' component terms under
    - |t|='1.0.'
  - 4) Exclude 'all' component terms under|t|='2.0.'

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

5) Property prediction ([Property Prediction] window)

🤡 INTERGL	AD 7 : Property Pr	ediction				
File Help						
8 🗟 [	?) 🔞 😒			INTER	GLAD7: Pro	operty Prediction
Regression	Equation					1
		Coefficient		С	iontent (massia)	
Component	Refractive Index (Ty			Initial	New	
SiO2	1.459E00				65.000 🔺	\
B203	1.455E00				10.000 =	
MgO	1.593E00				5.000	Glass-Forming Region
CaO	1.795E00			1	4.000	1
Na20	1.122E00				7.000	/
K20	1.335E00				5.000 🚽	
Component	Refractive Index (Ty			Initial	New	
SiO2*B2O3	-2.030E-02				0.065 🔺	
SiO2*CaO					0.026 🚍	
SiO2*Na2O	7.018E-01				0.045	Calculate
0100#1/20	4 001E 01				0.022 -	Clear New Content
			Total	0.000	100.000 %	
Property				~		Reset
					、 、	
	Specified		Predictive V	alue	)	
<ul> <li>Refrac</li> </ul>	tive index (Typical)			1.512		
-						
-						Close

- Return to the [Data List for Regression Analysis] window, and open the [Property Prediction] window from the [PROP] icon.
- Enter component values (SiO<sub>2</sub> 65%, B<sub>2</sub>O<sub>3</sub> 10%, MgO 5%, CaO 4%, Na<sub>2</sub>O 7%, K<sub>2</sub>O 5% Al<sub>2</sub>O<sub>3</sub> 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.

## 11. Composition optimization by linear multiple regression equations - Soda alumino-silicate glass with specified properties

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

- ${<}\mathrm{Refer}$  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)  $\rightarrow$  Search



• Specify a wide composition condition to collect many related data. For example set up composition conditions as follows.  $10 \leq SiO_2 \leq 90\%$ ,  $1 \leq Al_2O_3 \leq 25\%$ ,

 $1 \leq Na_2O \leq 25\%, \ SiO_2+Al_2O_3+Na_2O \geq 90\%$  (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)

🥝 INTE	RGLA	D 7 : Data List (	lor Regression An	alysis						
File To	ools H	elp								
4	<b>2</b>	I 🗟 🖨 🔮	🛱 🛃 🗵 🔛		: : :	6	INTEF	GLAI	0 7: Regressio	on Analysis
						Detail				
	-	Testal March 1	40							
	9	Total Number	43 Compo	nent Un	it mass to 🔹	informati	on		<u> </u>	_
		Number of Sourc	es 18 Prop	erty Un	it Common 💌			Compo	nent Analyze	
Delete	No.	Glass No.	Data Source	Year	Data Source Number	Si02	AI203	Na2O	Expansion Coeff (19 (10-7/K)	Expansion Co (Predictive V
	1	GJ02-015829	J. Non-Crystalline S	1977	v.026, p.0517	75.89	1.15	13.67	7.900E+01	
	2	GJ02-032267	J. Austral. Ceramic .	1984	v.020, p.0053	74.57	1.56	14.22	8.690E+01	
	3	GJ02-032270	J. Austral. Ceramic .	1984	v.020, p.0053	73.67	1.56	14.82	8.960E+01	
	4	GJ02-032271	J. Austral. Ceramic .	1984	v.020, p.0053	73.46	1.56	15.13	9.050E+01	
	5	GJ02-032272	J. Austral. Ceramic .	1984	v.020, p.0053	73.36	1.56	15.43	9.140E+01	
	6	GC05-051160	Schott AG (DE)		8329	84.00	3.00	3.00	2.750E+01	
	7	GC02-051349	Corning Inc (US)		0080	73.00	1.00	17.00	9.350E+01	
	8	GC02-051362	Corning Inc (US)	1976	0317	61.00	17.00	13.00	8.800E+01	
	9	GJ02-055405	Glastech. Ber.	1980	v.053, p.0149	63.38	12.03	24.58	1.210E+02	
	10	GJ06-055406	Glastech. Ber.	1980	v.053, p.0149	62.04	15.69	22.26	1.090E+02	
	11	GJ06-055407	Glastech. Ber.	1980	v.053, p.0149	61.67	18.88	19.45	1.000E+02	
	12	GJ06-055408	Glastech. Ber.	1980	v.053, p.0149	60.36	23.08	16.55	9.200E+01	
	13	GJ06-055409	Glastech. Ber.	1980	v.053, p.0149	59.94	24.20	15.86	8.850E+01	
	14	GJ06-082265	Glass Phys. & Cher	n. 1982	v.008, p.0121	65.26	15.63	9.47	7.500E+01	
	15	GJ06-082266	Glass Phys. & Cher	n. 1982	v.008, p.0121	66.19	16.52	10.05	7.500E+01	
	16	GJ06-082267	Glass Phys. & Cher	n. 1982	v.008, p.0121	66.70	17.11	10.40	7.200E+01	
	17	GJ06-082268	Glass Phys. & Cher	n. 1982	v.008, p.0121	68.74	19.44	11.82	7.000E+01	
	18	GB02-088942	Technical Glasses	1961	v.001, p.0265	70.94	1.14	21.29	1.030E+02	
	19	GB02-096094	Properties of Glass	1954	v.001, p.0232	72.12	8.95	18.77	8.110E+01	
	20	GB02-096095	Properties of Glass	1954	v.001, p.0232	72.22	6.87	20.67	9.390E+01	
	1	1	4		П	1				

• 43 glasses are listed.

### 3) Regression analysis by a linear equation

	-Selectiion of 1-Co If necessary, cf	mponent Term nange the follo	is wing con	dition : Apply	1
	Min. num. of gl	asses = 1 asses = 2	% of glas	total retrived glas ses to one compo	ses ner
	Select All C	Component	Clear	All Component	
	Component	Number of	Glasses	Max. Content %	
2	SiO2		43	84.110	
r	AI2O3		43	24.430	
r	Na2O		43	24.580	
V	B203		3	10.000	
v	MgO		7	4.000	
2	CaO		27	9.950	
	BaO		1	1.940	
2	LI20		5	3.390	
r	K20		6	6.540	
r	BeO		4	9.310	
V	ZnO		2	6.080	
	SrO		1	1.050	
	Cr2O3		1	0.320	
2	Fe2O3		14	0.430	
	Sb2O3		1	0.200	
¥	TIO2		5	5.690	
2	803		3	0.250	
	F		1	4.130	
	BACK	Next	ок	Cancel	

QUESTION
Scloetion of Explanetacy Variables in Multiple Regression Analysis:     1.Component Terms: 0     3.Component Terms: 0     OK Cancel

- 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.

<b>a</b> 6	3 🗵	🝸 🞯 🔞			INT	FERGLAD 7	: Regressio	on Analys
Proper	ty							
20	10 Refra	tive Index (Typic	al) ( Common )		Exe	ecute Verify	Result	
Analys	is Conditi	on		Select Comp	onents	~ ~		
Anabesi	is Method	y=Σa.x.+k				01		
rindiyo	is method			Select All C	omponent	Clear All Compo	nent	дрру
			xx ≥x ≥ 99 ▼%	Exclude of	component terms	s less than 3	data	
variabl	e y:	🖲 y 🔾 1/y	🔾 log y	Exclude	2-&3- Comp	onent terms und	er  t = 0.0 💌	
						Component	h luur h eu	Component
Select	c	omponent	Coefficient	Std. Error	tValue	vs Property	Number	vs Property
						Correlation	of Data	Correlation Plot
<b>r</b>	8102	/	1.46602E00	0.005	270.165	-0.47664	43	Figure
V	AI203	/	1.50377E00	0.011	142.807	0.12083	43	Figure
V	Na20		1.61568E00	0.019	87.177	0.24936	43	Figure
2	B2O3		1.50262E00	0.048	31.585	-0.55167	3	Figure
V	MgO		1.58360E00	0.100	15.911	0.06615	7	Figure
r	CaO		1.75977E00	0.026	67.881	0.40293	27	Figure
~	Li20		2.15029E00	0.118	18.180	0.35606	5	Figure
~	K20		1.68227E00	0.205	8.222	0.26234	6	Figure
×	BeO		1.73941E00	0.048	36.353	0.30557	4	Figure
×	ZnO	1	1.65908E00	0.087	19.168	0.14678	2	Figure
r	Fe2O3		-4.31762E-01	2.759	-0.156	0.11591	14	Figure
×	TiO2		1.84356E00	0.093	19.798	0.27654	5	Figure
2	803		7.76641E00	8.536	0.910	0.06029	3	Figure
	Xx		-3.18588E00	6.604	-0.492			Figure



- 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<sub>2</sub>O<sub>3</sub> with -0.156, SO<sub>3</sub> with 0.910, and execute again. Then all the |t| values become ≥ 2, and R<sup>2</sup> is 0.9209. By this operation the regression equation of refractive index is completed.
- INTERGLAD 7 File Tools Help INTERGLAD 7: Regression Analysis 🖬 🗃 🗹 📝 🔞 🕼 1020 Exp Execute Verify Re ult Coeff (Typical) ( Cor reie Condi Analysis Method : ○ y=∑a,x,+ Select All Co Clear All Co Apply o y=Σa,x,+a,x, Exclude c ariable 🖲 y 🔾 1/y 🔾 log y Excl 
   E
   SIO2

   E
   A1203

   E
   Na20

   E
   B203

   E
   Ca0

   E
   Ca0

   E
   L120

   E
   Be0

   E
   Zn0

   E
   Fe203

   E
   TO2

   E
   S033

   Xx
   Nx
   5060E01 5.719 -0.45276 .75987E0 -0.00193 0.87370 Figure Figure 19.533 -7.44011E01 50.13 1.48 -0.6722 8.40238E0 104.893 27.322 0.8 -0.01947 1.29383E0 4.736 0.0100 -0.28703 2.69079E0 2.37011E0 124.653 2.159 215.648 50.427 91.223 2907.728 2.83975E0 0.563 0.21134 6 88894ED 0.14531 Figure Figure -6.90206E0 1.05108E0 98.136 0.1359 Figure 02863E04 8995 748 0.00776 Figure 0916E04 6959.99
  - Next execute the regression analysis in the [Execution of Regression Analysis] window of thermal expansion in the same manner.

- 🗃 🕐 🙋 😫 INTERGLAD7: Regression Analysis 0.9613 Std. Error 1.110E+01 4.984 5.19 1.902E+01 -1.484 5.760E+0 7.440E+0 5.014E+01 8.402E+0 .049E+02 8.010E-0 1 294E+f 732E+0 4.736 .247E+0 2.691E+ 7.552E-0 Detai Delete lete a So Undo ale Linear Clo
- 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.'
  - 2) Exclude 'all' component terms under|t|='1.0' again.

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

Finally all the |t| values become  $\geq 2.0$ , and R<sup>2</sup>=0.9017. The regression equation is completed.

4) 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): 80×10<sup>-7</sup>/°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 SiO<sub>2</sub> content and decreasing

 $Al_2O_3$  and  $Na_2O$  contents with high regression coefficients of thermal expansion.

 An optimized composition is as follows: SiO<sub>2</sub> 67.88%, Al<sub>2</sub>O<sub>3</sub> 18.25%, Na<sub>2</sub>O 13.87%. This glass has 79.95×10<sup>-7</sup>/°C of thermal expansion coefficient and 1.493 of refractive index.

# 12. Investigation of correlation between composition and structure $-SiO_2$ content and bridging oxygen fraction

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

😓 INTERGLAD 7 : Search Structure Data							
File Tools Help							
🗃 🖬 🔮 🝸 😝 💗 🛶	INTEF	RGLAD 7: Glass Structure					
State Not Specified  Composition	_	DB Site					
O mass% @ mol% O at% Periodic Table	Clear Component Numerical	llear Data					
Main Component Component	Component Component %min %max						
AND V OR	OR OR	Charles Durdam					
		Glass System					
	OR OR -	AND V					
0 - % =< Total of Main Components							
Structure							
Description	Element Unit Value Min Value Max						
BO / [total O]	SH0-Si						
AND							
Measurement Method	Measurement Condition						
IR - Visible Visible - UV Lumines / IR - Visib	le Lumines / Visible - UV Temperature						
Raman NMR Moessbauer	XPS ESR X-ray						
Neutron XAFS Calc (MO,MD,etc)	Others	Glass ID					
Data Source							
AND -		1000					
		Max Data 1000					
First Author  Reset							

- 1) Specification of search conditions ([Search Structure Data] window)  $\rightarrow$  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) Searh result ([Data List of Structure] window)

🔆 INTERGLAD 7 : Data List of Structure										
File Tools Help										
🖙 🗃 🖬 🛱 💭 🏨 🗒 🖉 🧉 🖉 🚺 INTERGLAD 7: Glass Structure										
Data Source List Detail Information Component							Component	1		
Total Number 23 Component Unit mol%  Delete +, -, +, /						, ., ^, /	Property			
Number of Sources 3 Undo Structure								Structure		
Delete	No.	Glass No.	Data Source	Year	Data Source Number	BO / [total O] (AI-O-AI) (%)	BO / [total O] (SI-O-B) (%)	BO / [total O] (SI-O-AJ) (%)	BO / [total 0] (SI-O-SI) (%)	>
	1	8-00503	Phys. & Chem. Gla	1990	v.031, p.0030		1.0005-01		4.500E+01	1
	2	8-00504	Phys. & Chem. Gla	1990	v.031, p.0030		2.500E+01		5.500E+01	
	3	8-00505	Phys. & Chem. Gla	1990	v.031, p.0030		5.0		6.000E+01	
	4	S-00506	Phys. & Chem. Gla	1990	v.031, p.0030		6.0		6.000E+01	
	5	8-00507	Phys. & Chem. Gla	1990	x.031, p.0030		5.0		6.000E+01	
	6	8-00549	J. Chem. Soc. Japan	1981	v.089, p.0599				7.840E+01	
	7	8-00550	J. Chem. Soc. Japan	1981	v.089, p.0599				3.610E+01	
	8	S-00552	J. Chem. Soc. Japan	1981	v.089, p.0599				5.570E+01	
	9	8-00553	J. Chem. Soc. Japan	1981	v.089, p.0599				6.250E+01	
	10	8-00554	J. Chem. Soc. Japan	1981	v.089, p.0599				6.650E+01	1
	11	8-00555	J. Chem. Soc. Japan	1981	v.089, p.0599				5.670E+01	
	12	8-00556	J. Chem. Soc. Japan	1981	v.089, p.0599				6.800E+01	
	13	8-00557	J. Chem. Soc. Japan	1981	v.089, p.0599				7.480E+01	
	14	8-00558	J. Chem. Soc. Japan	1981	v.089, p.0599				6.760E+01	
	15	S-00559	J. Chem. Soc. Japan	1981	v.089, p.0599				6.380E+01	I
	16	8-00560	J. Chem. Soc. Japan	1981	v.089, p.0599				5.760E+01	
	17	8-00561	J. Chem. Soc. Japan	1981	v.089, p.0599				4.940E+01	I
	18	S-00754	Fall Meet. Ceram. S	1993	v.001, p.0078			6.520E+01	3.490E+01	I
	19	S-00756	Fall Meet. Ceram. S	1993	v.001, p.0078	1.380E+01		6.200E+01	1.370E+01	1
	20	8-00757	Fall Meet. Ceram. S	1993	v.001, p.0078	2.050E+01		4.100E+01	1.860E+01	I
	21	S-00758	Fall Meet. Ceram. S	1993	v.001. p.0078			6.280E+01	2.480E+01	1

- 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 SiO<sub>2</sub> 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 SiO<sub>2</sub> content.

# 13. Investigation of correlation between structure factors $-Q^2$ and non-bridging oxygen fraction of alkali-silicate glasses

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

MINTERGLAD 7: Search St	ructure Data			📃 🗆 🖾				
File Tools Help								
🗃 🖬 🗃 👩 🔞 🔞	4		INTE	RGLAD 7: Glass Structure				
State Not Specified 🛛 💌				DB Site				
Composition				✓ INTERGLAD Data				
0								
O massing @ more O atte	Periodic Table	Clear Component	La Numerical	lleer Data				
Main Compone	nt Component	Component	Component %min %max	Userbata				
AND V	OR	OR OR						
	OR	OR OR		olass system				
	OR			Alkali Silicate				
AND V	OR	OR OR		AND				
				AND *				
0 % =< Total of Main Co	mponents							
Structure								
1	- Hen	Element	Init Value Min Value May					
Q2/total X	icity in the second s	Liemen						
AND VIEW NB0 / [total 0]	<u> </u>							
AND								
Measurement Method			Measurement Condition					
D ) Seikle D) Seikle 10(	Luminos (10. Maible		feible 101					
Daman NMD	Moonehouer		Temperature					
Naman NATE	Cole (MO MD etc)	Others	Pressure	Class ID				
Neutron XAFS	Caic (MU,MD,etc)	Uthers		Glass ID				
Data Source								
AND 🔻				May Data 1000				
First Authors								
First Author				Search Reset				

- 1) Specification of search conditions ([Search Structure Data] window)  $\rightarrow$  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 Q<sup>2</sup> fraction in tetrahedra XO<sub>4</sub>. 'NBO/ [totalO]' means fraction of non-bridging oxygen to the total

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

🕼 INTERGLAD 7 : Data List of Structure												
File Tools Help												
🐱 🗃 🖬 🗟 🗮 💭 🕮 💭 🕼 🍯 🚱 INTERGLAD 7: Glass Structure												
Data Source List						Detail	Information	Componen	Component			
Total Number 37 Component Unit mo				Init mol% 💌	Delete	+, ., ^, /	Property					
Number of Sources 5			5			Undo		Structure				
Delete	No.	Glass No.	Data Source	Year	Data Source Number	(0) (%)	NBO / [total O] (SI-O) (%)	NB0 / [total O] (Ca-0) (%)	NB07T (Ei			
	1	S-00119	J. Non-Crystalline S	2002	v.297, p.0220	2.860E+01			-			
	2	8-00120	J. Non-Crystalline S	2002	y.297, p.0220	4.010E+01						
	3	S-00121	J. Non-Crystalline S	2002	v.297, p.0220	5.490E+01						
	4	S-00122	J. Non-Crystalline S	2002	v.297, p.0220	2.860E+01						
	5	8-00123	J. Non-Crystalline S	2002	y.297, p.0220	2.860E+01			_			
	6	S-00662	J. Material Science	1993	v.028, p.3473	8.220E+01						
	7	S-00663	J. Material Science	1993	v.028, p.3473	8.230E+01						
	8	8-00664	J. Material Science	1993	v.028, p.3473	7.030E+01						
	9	S-00665	J. Material Science	1993	v.028, p.3473	5.110E+01						
	10	S-01150	J. Jpn. Inst. Metals (J)	1983	v.047, p.0382	4.500E+01			-			

• 37 glasses of 5data sources are listed.

oxygen.

• 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<sup>2</sup> and NBO ([XY Plot] window)







- An XY Plot of Q2/totalX(Si) vs. NBO/ [totalO](O) is shown.
- With increasing Q<sup>2</sup>, 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 Q4/totalX(Si) vs. NBO/ [totalO](O) is shown.
- The figure shows a reasonable tendency that NBO fraction decreases with increasing Q<sup>4</sup>.

 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 Li<sub>2</sub>O+Na<sub>2</sub>O+K<sub>2</sub>O vs. NBO/ [totalO](O). It is found that the NBO fraction increases proportionally with increasing the alkali content.