Examples of Use

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[Search and Analysis of Structure Data]

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14. Investigation of correlation between structure factors

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

Notes

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

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

- 2) Refer the User's Manual for detailed operation. The corresponding 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.8.2.0.2 of INTERGLAD (with GP_42_2020.mdb and GS_37_2020.mdb) is used for these examples.

Search and Analysis of Property Data

 Search with a complicated composition – Thermal expansion coefficient of phosphate glasses Search thermal expansion coefficient data of phosphate glasses with Al₂O_{3 of} 10-20 mass%, containing Na₂O or K₂O, 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



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

🏷 INTE File To	RGLAD	8 : Data List of Pro	perty						-		×
ب	2	38			;	6		INTER	GLAD 8: Glas	s Prop	erty
		Data Sourc	e List			Detail		Information	Component		
	0	Total Number	258 Compo	nent U	nit mass% 💌	Delete		* *. l	Property		
		Number of Source	ces 66 Proj	perty U	nit Common 💌	Undo	Ad	ditivity Equation	Structure		
Delete	No.	Glass No.	Data Source	Year	Data Source Number	AI203	Na29	K20 Expanse	ion Coeff (Ty 18-7/K)		
	1	GP20-035418	Japanese Patent	1986	A036137	12.16	4.22		868E+01		
	2	GP20-037218	Japanese Patent	1982	A129841	15.60	5.50		1.29E+02		
	3	GJ20-045104	J. American Cerami	1981	v. 064 p. 0206	17.00		2.25	7.44E-01		
	4	GJ20-045105	J. American Cerami	1981	v. 064 p. 0206	7.22		4.34	6.67E+01		
	5	GC20-051404	Corning Inc. (US)		4602	14.00	0.89		5.4E+01		
	6	GP20-065115	Japanese Patent	1987	A235231	11.21		8.22	9.8E+01		
	7	GP20-065117	Japanese Patent	1987	A235231	11.71		13.70	1.07E+02		
	8	GP20-065120	Japanese Patent	1987	A235231	10.93		15.53	1.05E+02		
	9	GP20-065121	Japanese Patent	1987	A235231	10.02	1.10	12.17	1.18E+02		
	10	GP20-065122	Japanese Patent	1987	A235231	10.13	3.33	8.94	1.08E+02		
	11	GP20-065123	Japanese Patent	1987	A235231	10.06		8.88	1.23E+02		
	12	GP20-065124	Japanese Patent	1987	A235231	11.83	1.02	7.44	1.09E+02		
	13	GP20-065125	Japanese Patent	1987	A235231	11.80	1.02	7.42	1.09E+02		
	14	GP20-067932	Japanese Patent	1981	A051574	10.00		5.00	9.8E+01		
	15	GP20-067938	Japanese Patent	1981	A051574	10.00		5.00	8.3E+01		
	16	GB20-087441	Glass Hand Book (J)	1975	v. 001 p. 0136	17.00	18.00	11.00	1.55E+02		
	17	GP20-094216	US Patent	1985	A4544974	12.05	15.38		1.25E+02		
	18	GP20-094218	US Patent	1985	A4544974	11.41	15.60		1.2E+02		
	19	GP20-102250	Japanese Patent	1989	A242440	13.50		1.00	6.7E+0		
	20	GP20-102251	Japanese Patent	1989	A242440	18.00		2.20	6.8E+01		
	21	GP20-102253	Japanese Patent	1989	A242440	16.00	1.20		6.42+01		
	22	GP20-104214	Japanese Patent	1990	A240282	10.17	10.81		1/5E+02		
	23	GP20-104216	Japanese Patent	1990	A240283	10.63	\$ 38		1.15E+02		
	24	GP20-106418	LIS Patent Schott	1000	44020397	10.10	2 27	\sim	1 107E+02		

- Open the [Search Property Data] window by clicking the [Search Property Data] button in the [Main] window, select the [Detail Search] tub, and specify search conditions.
- Select '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 the simultaneous selection of Na₂O and K_2O is not available on the periodic table.
- Cr Oxides can be selected by selecting 'Cr: 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] column. The selection of 'Linear Expansion Coeff' (a middle category item, boldtype) brings the same result.
- Take notice of 'Total Number' of the Data Source, 258.
- A table with values of components, property data etc., which are specified as the search conditions, appears.

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

DINT 😒	ERGLA	D 8 : Data List of Prop	perty						-		×
File Te	pois F	Help			1 9 8 7	6		INTER		e Pror	nerty
		Data Source	List	and a		Detail	Inform	ation	Component	SFIO	ferty
		Total Number	258 Compo	nent Ur	iit mass% 💌	Delete	•	•,1	Property		
		Number of Source	s 66 Prop	erty Ur	tit Common 💌	Undo	Additivity	Equation	Structure		
Delete	No.	Glass No.	Data Source	Year	Data Source Number	AI203	Na20 K2	Expansio (10	n Coeff (Ty I-7/K)		- H
	5	GC20-051404	Corning Inc. (US)		4602	14.00	0.89		5.4E+0		-
	162	GI20-191886R	NGF's Additional N	2001	v. 004 p. 0009	10.26	4.00E		5.617E+01		-
	69	GP20-125149	US Patent Schott	1992	A5173456	13.33	2.0	11	5.934E+01		
	85	GP20-125482	European Patent	1992	A0492577	13.33	2.0	1	5.934E+01		
	135	GP20-154889	Japanese Patent	1994	A040743	11.96	1.8	0	5.934E+01		

e roois neip							
S 🖓 🚺	0					INTERGLAD	3: Glass Prope
lass No.		State	Prop	erties			
GC20-05	1404	Glass	ID	Specified	Value	Unit	Condition
001000			0510	Density at RT	2520.0	kg/m3	
omposition			0540	Young's Modulus at RT	7.096E10	Pa	
Condition of Data		Glass System	1021	Expansion Coeff (0~300C)	54.0	10-7/K	
Target		Phosphate	1113	T at 1E4 dPa.s (Working P)	1306.0	к	
Components		Alumino-Silicate	1116	T at 1E7.6(7.65) dPa.s (Sof P)	1033.0	к	
			1119	T at 1E13 dPa.s (Annealing P)	833.0	к	
1 1	10.07		1122	T at 1E14 dPa.s (Strain P)	792.0	к	
3IU2	14.00	Filler / Crystal / Substrate	2018	Refract Index 589.3nm D	1.51		
AI203	14.00	/ Ratio Shape	5010	Water Durability Other	3.0		
120	0.20		5011	Water Durability ASTM	3.0		
Na20	0.09						-
FeO	1.29						
2n0	4.1/	- Pol Col Motorial	Autho	ors			
SILO	2.08 -	Sol-del material					
Commercial Glass	5		Data	Source			
Corning A	602		Corni	ng Inc. (US)			
corning 4	OOL		4602				
ppearance, Featu	re, Process	Usage	Mem	0			
		Wavelength Selector					
			Note				
			Heat	Absorbing			

[Detail Data of Property] window

🍅 IN	ITERGLAD 8 : Data Source Lis	t			-		×	(
File	Tools Help							
	a 🖓 🕐 🕼			INT	ERGLAD 8: Data	source	Li	st
	Data Source	Year	Data Source Number	Author	Memo	Num of D	Jata	
1	Physics and Chemistry o	1997	Vol. 038 Page 0015	Montagne L., Palavit G.,		/	10	^
2	J. Materials Science	1997	Vol. 032 Page 5851	Donald I.W., Metcalfe B.L			70	Λ
3	European Patent	1990	A0356746				58	Ν
4	US Patent	2013	A0330600		Claim: 35-50mol%P2O5		8	1
5	J. Non-Crystalline Solids	2001	Vol. 288 Page 0008	Karabulut M., Melnik E., S	Melting : in alumina crudi		11	
6	US Patent	2017	A9539665		Claim: 35-50mol%P2O5,		8	
7	US Patent	2004	A6784128				10	
8	Japanese Patent	2007	A290886				10	
9	Data Book of Glass Com	1991	Vol. 001 Page 0120				5	
10	Glass Physics & Chemis	2004	Vol. 030 Page 0425	Batyaev I.M., Leonov A.V.	Melting : in alundum cru		1	
11	US Patent	1992	A5173456				61	
12	European Patent	2003	A1275622				10	
13	Glass Technology	1991	Vol. 032 Page 0166	Peng Y.B., Day D.E.			26	
14	Japanese Patent	1994	A107428				8	
15	J. American Ceramic Soc.	1981	Vol. 064 Page 0206	Abe Y., Kawashima K., S			2	
16	Japanese Patent	1981	A051574				10	1
17	US Patent	2003	A0153450				10	1
18	US Patent	2005	A0159291				8	1
19	J. Non-Crystalline Solids	1997	Vol. 222 Page 0396	Brow R.K., Tallant D.R.			2	-
			CI	ose		\sim	/	

[Data Source List] window

- Sort 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 expansion coefficient of the lowest value can be found. The detailed data of a glass can be checked by selecting its row and clicking the [Detail] button.

- 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.

• If necessary, analyze the result using Ternary Plot or XY Plot.

2. Ternary plot analysis of property data

- Thermal expansion coefficient of SiO₂-Na₂O-TiO₂ glasses

 $Investigate\ relation\ between\ composition\ and\ thermal\ expansion\ coefficient\ on\ SiO_2-Na_2O\ -TiO_2\ glasses.$

<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)
 - \rightarrow Search



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

File To	ols H	elp	<u> </u>												ĺ
4	2	I 🗟 🛎 🔤		1			?	6		1	NTERG	LAD 8:	Glass	s Prop	er
	[Data Source	List					Detail		Informa	tion	Compor	ent		
	Ó	Total Number	234	Compor	nent Un	it mass%	- 1	Delete		1.55	1	Proper	rty		
	[Number of Source	s 41	Prop	erty Un	it Common	-	Undo	Add	litivity Ec	uation	Structu	ire		
Delete	No.	Glass No.	Data So	ource	Year	Data So Numb	urce er	SiO2	Na2O	TiO2	Expansion (10	n Coeff (Ty I-7/K)			
	1	GB02-006032	Handbook o	f Glass	1986	v. 001 p. 016	3	67.08	15.21	17.71		8.4E+01			
	2	GB02-006033	Handbook o	f Glass	1986	v. 001 p. 016	3	51.85	15.56	32.58		1.1E+02			
	3	GB02-006034	Handbook o	f Glass	1986	v. 001 p. 016	3	49.04	20.56	30.40		1.12E+02			E.
	4	GB02-006035	Handbook o	f Glass	1986	v. 001 p. 016	3	35.56	20.57	43.87		1.08E+02			1
	5	GB02-006036	Handbook o	f Glass	1986	v. 001 p. 016	3	42.29	21.44	36.27		1.16E+02			
	6	GB02-006037	Handbook o	f Glass	1986	v. 001 p. 016	3	69.61	23.39	6.99		1.1E+02			
	7	GB02-006038	Handbook o	f Glass	1986	v. 001 p. 016	3	50.68	22.51	26.81		1.07E+02			1
	8	GB02-006039	Handbook o	f Glass	1986	v. 001 p. 016	3	30.71	22.63	46.66		1.15E+02			1
	9	GB02-006040	Handbook o	f Glass	1986	v. 001 p. 016	3	58.00	25.69	16.31		1.18E+02			

3) Ternary plot



- Select '90' mass% as the minimum Total of Main Components, SiO₂, Na₂O and TiO₂.
- Select 'Expansion Coeff (Typical)' for the Specified of the [Property] column.

 \bullet 234 glasses are searched.

- Open the [Ternary Plot] window by clicking the [Ternary Plot] icon. Select SiO₂, Na₂O and TiO₂ for the 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. ○ indicates 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 the 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 100.4×10⁻⁷/K, and the ternary diagram with SiO₂ (100%), Na₂O (50%), TiO₂ (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>

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



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

🔯 INTE	RGLAD	8 : Data List of Prop	erty						-		\times
File To	ols H	elp	-								
4	2	88			1 🧝 📰 🕐	6		INTERGL	AD 8: Glas	s Prop	perty
		Data Source	List			Detail	Info	rmation	Component		ŕ
	\subseteq	otal Number	3399 Compo	nent Ur	nit mol% 💌	Delete	•	, , *, 1	Property		
	,	lumber of Sources	2293 Prop	erty Ur	nit Common 💌	Undo	Additiv	ty Equation	Structure		
Delete	No.	Glass No.	Data Source	Year	Data Source Number	Refract Inc	tex 587.6	Abbe Value (nd-	1)/(
	1	GJ05-008626	Glass Science and	1987	v. 060 p. 0234		1.502	6.56E	+01		-
	2	GJ05-008627	Glass Science and	1987	v. 060 p. 0234		1.502	6.62E	+01		
	3	GJ05-008628	Glass Science and	1987	v. 060 p. 0234		1.503	6.652E	+01		
	4	GJ05-008629	Glass Science and	1987	v. 060 p. 0234		1.502	6.665E	+01		
	5	GJ05-008630	Glass Science and	1987	v. 060 p. 0234		1.503	6.67E	+01		
	6	GJ05-008631	Glass Science and	1987	v. 060 p. 0234		1.503	6.659E	+01		
	7	GJ05-008632	Glass Science and	1987	v. 060 p. 0234		1.504	6.685E	+01		
	8	GJ05-008633	Glass Science and	1987	v. 060 p. 0234		1.504	6.722E	+01		

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



- Select 'Glass' in the [State] pulldown menu.
- 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' in the [Data Source] column.
- Select '5000' in the [Max Data] pulldown menu.

• 3399 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 3399 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
\rightarrow	Search



- Select 'Glass' for the State, and 'Boro-Silicate' for the Glass System.
- Select 'Viscosity 700C' for the Property, and check in the [Numerical] and the [Extension Search] checkboxes shown in the window example.

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

Dinte File To	RGLAD	8 : Data List of Pro	perty				-	o ×
ب	2	88		¥¥	6	INTERGL	AD 8: Glass	Property
		Data Source	e List	0	Detail Int	formation	Component	
		Total Number	1017 Com	ponent Unit mol% 💌	Delete	+, -, *,/	Property	
	<	Number of Source	es 205 P	roperty Unit Common 👻	Undo Additi	ivity Equation	Structure	
Delete	No.	Glass No.	Data Source	Year Data Source Number	Viscosity at 700C (dPa.s)			
	1	GJ02-000026	Glass Science and	1983 v. 056 p. 0125				
	2	GB04-004679	Handbook of Glass.	1986 v. 001 p. 0299				1
	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. American Cerami	1980 v. 063 p. 0126	2.0E+10			
	9	GJ05-010069	J. American Cerami	1974 v. 057 p. 0109				
	10	GJ05-010070	J. American Cerami	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	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			

3) Data interpolation or extrapolation

🔯 Select Data Interpolation Condition 🛛 🕹 🗙
Specify interpolation method.
Property
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

- As the search result, all the boro-silicate glasses which have registered viscosity data at high temperatures are listed. 1017 glasses appear.
- Search of viscosity data at 700°C can be performed, also when the user selects the bold type item 'Viscosity(100-1000C).' In this case, all the glasses which have one or more numerical data of viscosity at 100-1000°C are listed. 551 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/ (absolute temperature). Then click the [OK] button.

🍅 INTE	RGLAD	08: Data List of Prop	perty					-	D X
4	-	138 8			黑黑 [2 😝 😫	INTER	GLAD 8: Glass	Property
	~	Data Source	e List			Detail	Information	Component	
		Total Number	1017 Com	ponent Uni	t mol%	Delete	*, -, *,/	Property	
		Number of Source	es 205 Pi	operty Uni	t Common	Undo	Additivity Equation	Structure	
Delete	No.	Glass No.	Data Source	Year	Data Source Number	Viscosi (di	ty at 700C Pa.s)		
	1	GJ02-000026	Glass Science and	1983 v.	056 p. 0125				-
	2	GB04-004679	Handbook of Glass.	. 1986 v.	001 p.0299	1			5
	3	GB04-004680	Handbook of Glass.	. 1986 v.	001 p. 0299	1	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. American Cerami	1980 v.	063 p.0126		2.0E+10		
\triangleleft	9	GJ05-010069	J. American Cerami	1974 v.	057 p.0109	\rightarrow	7.973E+07		
	10	GJ05-010070	J. American Cerami	1974 v.	057 p. 0109		7.311E+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+07		

- The 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 ± 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 plotpoints appear in red-purple color. The style of plotpoints and axis-scales can be changed by the pulldown menus on the bottom of the graph.

5. Search commercial glasses – High strength glass fibers for FRP Investigate high strength glass fibers 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)
 - \rightarrow Search



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

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

Dinter 🏷	RGLAE	8 : Data List of Prop	perty						-		×
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4	2	I 😒 🛎 💿	倉 🤮 🕌 🗮	닕		1 😺 🗊	IN	TERGLAD	8: Glass	s Prop	erty
		Data Source L	ist			Detail	Informatio	n Con	ponent		^
	\triangleleft	Total Number	18 Compon	ent Unit	mol% 💌	Delete	+,-,*,/	Pr	operty		
	ſ	Number of Sources	s 18 Prope	erty Unit	Common 👻	Undo	Additivity Equa	ation Str	ucture		
Delete	No.	Glass No.	Data Source	Year	Data Source Number	Young	s Modulus at Te	ensile Strength (MPa)	>		
	10	GC06-052346	Nitto Boseki (J)	1	NITTOBOT-GLAS	S		4.655E+03			
	4	GC06-052225	Owens Corning (US) 1989	S-Glass		8.55E+01	4.585E+03			
	3	GC03-052224	Owens Corning (US) 1989	E-Glass	-	7.235+01	3.445E+03			
	6	GC03-052249	Asahi Fiber Glass (J)	E-Glass		7.252E+01	3.43E+03			
	7	GC03-052250	Asahi Fiber Glass (J)	ECR-Glass		7.223E+01	3.43E+03			
	9	GC03-052344	Nitto Boseki (J)		NITTOBOE-GLAS	s		3.43E+03			-
	5	GC03-052226	American Biomateri	1989	C-Glass		6.89E+01	3.31E+03			
	12	GC02-052349	Nitto Boseki (J)		NITTOBOC-GLAS	8		3.087E+03			
	11	GC05-052348	Nitto Boseki (J)		NITTOBOD-GLAS	S		2.254E+03			
	8	GC05-052262	Central Glass (J)		E-GLASSFIBER		7.252E+01	1.96E+03			
	13	GC03-052753	PPG Industries (US)		FIBER GLASS			1.7E+03			
	2	GC03-052074	Nippon Sheet Glas		E-Glass		7.35E+01	1.47E+03			
	14	GC03-071205	Nippon Electric Gla.	. 1989	EF		7.252E+01	1.47E+03			
	1	GC03-051554	Corning Inc. (US)		E-Glass		7.4E+01				
	15	GC05-071206	Nippon Electric Gla.	. 1989	D-40						
	16	GC03-144895	Saint-Gobain (FR)	1983	02418						
	17	GC06-144896	Saint-Gobain (FR)	1983	0320180						H
	18	GC06-144897	Saint-Gobain (FR)	1985	02509						



3) Investigation of a searched glass



🤣 INTE	RGLAD	8 : Data List of	Property									- 0	×
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÷ (2	3 8		¥ 🖬		1 🧱 🖬 👔	6			1	NTERGLAD	B: Glass Pr	operty
	Data Source List							etail		formation	Component		
	Total Number 9 Component Unit m					ment Unit mass%	-	elete		1.11	Property)	
	Total Num Number of Nete No. Glass No.		nber of Sources	5 9	Prop	perty Unit Common		Jndo	Additivity Equation		Structure		
Delete	No.	Glass N	o. Data	Source	Year	Data Source Number	SiO2	AI2O3	MgO	Density at RT ((oung's Modulus (GPa)	Tensile Strengt	Expans
	1	GB06-00179	1 Handbook	of Glass	1986	v. 001 p. 0093	65.00	25.00	10.00	2.5			
	2	GJ03-03234	5 Glass Phy	sics & C	1980	v. 006 p. 0444	65.00	25.00	10.00	2.5			
	3	GC06-0515	55 Corning In	c. (US)		S-Glass	65.00	25,00	10.00				
	4	GC06-0522	25 Owens Co	ming (US)	1989	S-Glass	65.00	25.00	10.00	2.46	8.55E+01	4.585E+0	3
	5	GB06-1647	5 Fundame	tals of In	1994	v. 001 p. 0003	65.00	25.00	10.00				
	6	GJ06-17203	9 J. Non-Cry	stalline S	1997	v. 209 p. 0069	65.00	25.00	10.00				
	7	GB06-1747	2 Data Book	of Glass	1991	v. 001 p. 0134	65.00	25.00	10.00	2.49	8.624E+01	4.606E+0	
	8	GP06-2054	4 Japanese	Patent	2000	A233942	65.00	25.00	10.00	-			
	9	GP06-3000	17 European	Patent	2010	A2221335	65.00	25.00	10.00	<u> </u>		-	

- 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 fibers.
- By sorting the Tensile Strength column, glasses with high strength can be found. (NITTOBO T-Glass and S-Glass are the highest.)

- 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 after selecting 'mass%' for the Unit. Not specify 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 the [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



🧶 INTE	RGLAD	7 : Data List	of Property										
File To	ols He	dp 🖉											
4	2	9 8 9				2 🔮 😂					INTERGLAD	': Glass Prope	erty
		Da	ta Source List			[Detail		Informati	ion	Component		1
		Total N	umber 32	Somponent Unit	mas	5 💌	Delete		+, -, *,)	0	Property	>	
		Number	r of Sources 23	Property Unit	Com	110N 💌	Undo	Ade	ditivity Eq	uation	Channelson		
Delete	No.	Glass No.	Data Sc	urce	Year	Data :	Source	Si02	AI203	MaO	Young's Modulus at	Tensile Strength (MPa)	-
	V	GJ06-073521	Glass Phys. & Chem.	-USSR	1982	v.008, p.00	26	64.98	26.58	8.44	9.200E+01		-
	21	GJ06-073520	Glass Phys. & Chern.	USSR	1992	v.608, p.08	28	55.09	24.30	9.01	9.100E+01		
	30	GB06-174772	Data Book of Glasses	Composition (J)	1991	x.001, p.01	34	85.00	25.00	10.00	8.624E+01	4.606E+03	
	23	GB06-089932	Glass Hand Book (J)		1975	x.001, p.02	19	64.36	24.82	10.31	8.575E+01		
	18	GC06-052225	Owens Coming (US)		1989	S-Glass		65.00	25.00	10.00	8.550E+01	4.585E+03	
	1	GB06-001787	Handbook of Glass P	roperties	1986	v.001, p.00	93	63.00	25.00	12.00			-
	2	GB06-001790	Handbook of Glass P	roperties	1986	x.001, p.00	93	66.30	23.30	10.40			
	3	GB06-001791	Handbook of Glass P	roperties	1986	×.001, p.00	93	65.00	25.00	10.00			
	4	GB06-001792	Handbook of Glass P	roperties	1986	x.001, p.00	93	65.50	25.00	9.50			-

🧭 IN	TER	GLAD 7 : Glass	es from a	i Data So	urce			
File	Too	ls Help						
8	12 FL	🖁 🚑 [👩	6				INTERGLAD	7: Data Source
	Dat	a Source :	Glass	Phys. & Cl	hemUSSF	ર	Number of Data :	5
	Dat	a Source Number	: Vol. 0	08 Page O	026 (1982)		Component Unit	mass% 💌
	Aut	hor :	Aslan Gorba Fertik	iova M.S., D ichev V.V., iov V.I.	orzhiev D. Bystrikov	B., Sapozhkova L.A., A.S., Petrakov V.N.,	Property Unit	SI 💌
	Mei	mo :					De	tail
		Glass No.	SIO2	AI203	MgO	Vickers Hardness ((Pa)	Density at RT (kg/m3)	Young's Modulus at (Pa)
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
3		GJ06-073520	66.09	24.30	9.61	5.880E+09	2.485E+03	9.100E+10
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
		1						•
						Close		

[Glasses from a Data Source] window

- 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.

- 40 glasses of 26 data sources are listed. When patents are also included for the search condition, 119 glasses of 57 data sources are listed.
- List the values of 'Tensile Strength' and 'Young's Modulus at RT' from the [Property] button, and sort the Young's Modulus column. 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 glasses. All the data (5 glasses) in this data source can be checked.

Property Prediction by Additivity Equations

6. Property prediction of glasses with a specified composition - Boro-silicate glasses

Predict density, thermal expansion coefficient and refractive index of a boro-silicate glass 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)



2) Prediction of thermal expansion coefficient



- Open the [Additivity Equation for Property Prediction] window by clicking the [Property Prediction] button in the [Main] window and [Additivity Equation for Property] button. 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 [Component %] column. 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.
- 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 68.62×10^{-7} /K in the [Predictive Value] column.

3) Prediction of thermal conductivity



4) Prediction of refractive index



- Select 'Ammer (Silicate and Borate)' after developing 'Thermal Conductivity' in the [Predictive Equation] menu.
- By clicking the [Calculate] button, the predictive value 0.8968 W/(mK) (30°C) appears in the [Predictive Value] column.
- In this example, equations of 'Ratcliffe (Silicate)' and 'Russ (Silicate)' are also available, and 0.8349 W/(mK) (0°C) and 0.9256 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>

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

7. 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) \rightarrow Search
 - Open the [Search for Regression Analysis] window by clicking the [Property Prediction] button and then the [Multiple Regression Analysis] button in the [Main] 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 ([Select Component Terms] dialog boxes)

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						Detail			-
		tal Number	535 Compone	nt Unit	mol% In Common	formation +,	-,*,/	10	
	-		Proper	(y onic	Data Source	Density at RT	Density at RT	Density a	a =
Delet	e No.	Glass No.	Data Source	Year	Number	(g/cm3)	(Predictive Value)	(Residu	18
	1	GB02-000500	Handbook of Glass	1986	v. 001 p. 0065	2.74			
	2	GB02-000501	Handbook of Glass	1986	v. 001 p. 0065	2.867			E
	3	GB02-000502	Handbook of Glass	1986	v. 001 p. 0065	2.99			
	4	GB02-000503	Handbook of Glass	1986	v. 001 p. 0065	3.115			
	5	GB02-000504	Handbook of Glass	1986	v. 001 p. 0065	2.405			
	6	GB02-000505	Handbook of Glass	1986	v. 001 p. 0065	2.51			
	7	GB02-000506	Handbook of Glass	1986	v. 001 p. 0065	2.636			
	8	GB02-000507	Handbook of Glass	1986	v. 001 p. 0065	2.885			
	9	GB02-000508	Handbook of Glass	1986	v. 001 p. 0065	2.439			-

[Selectiion of 1-Con	nponent Terms		1
	If necessary, cha	ange the following co	ndition : Apply	
	🖌 Min. num. of gla	sses = 1 % d	of total retrived glasses	
	🗹 Min. num. of gla	sses = 2 gla	isses to one componen	t
	Calant All C	Clas	All Component	
	Select All Co	Clea	ir All Component	
_	Component	Number of Glasses	Max. Content %	
2	SiO2	47	0 85.000	
*	B2O3	17	3 50.000	
2	AI2O3	20	7 25.000	
2	MgO	3	0 30.000	
V	CaO	12	3 38.200	
*	BaO	7	3 30.000	
2	Li2O	3	3 35.000	
×	Na2O	17	7 40.000	
V	K2O	14	2 35.000	
v	MnO	4	5 45.000	
	FeO		1 0.540	
	CoO		2 1.790	
¥	CuO		5 3.140	
v	ZnO	47	5 70.000	
r	SrO	2	8 30.000	
	CdO		1 40.000	
2	PbO	2	5 40.000	
	SnO		0 0.000	
		· · · · ·		

- \bullet 535 glasses (147 data sources) are listed.
- Open the [Select 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 1component Terms at the 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.

QUESTION	×
Selection of Explanatory Variables in M 1-Component Terms: 31 2-Component Terms: 0 3-Component Terms: 0	ultiple Regression Analysis:
OK Cancel	

1-Component Terms: 31.

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							Detail	_							*
							Detail								
	To	tal Number	535	Compone	nt Unit	mol% 💌 I	nformation	1	*,-,*,	,1		_			
	Nu	mber of Sources	147	Proper	ty Unit	Common 💌			Compon	ent 🤇	Analy	te			
Delete	No.	Glass No.	Da	a Source	Year	Data Source Number	SiO2	B2O3	AJ2O3	MgO	CaO	BaO	Li2(-
	1	GB02-000500	Handbo	ok of Glass	1986	v. 001 p. 0065	65.00						15.		
	2	GB02-000501	Handbo	ok of Glass	1986	v. 001 p. 0065	60.00						15.		
	3	GB02-000502	Handbo	ok of Glass	1986	v. 001 p. 0065	55.00						15.		
	4	GB02-000503	Handbo	ok of Glass	1986	v. 001 p. 0065	50.00						15.		
	5	GB02-000504	Handbo	ok of Glass	1986	v. 001 p. 0065	75.00						20.		
	6	GB02-000505	Handbo	ok of Glass	1986	v. 001 p. 0065	70.00						20.		
	7	GB02-000506	Handbo	ok of Glass	1986	v. 001 p. 0065	65.00						20.		
	8	GB02-000507	Handbo	ok of Glass	1986	v. 001 p. 0065	55.00						20.		
	9	GB02-000508	Handbo	ok of Glass	1986	v. 001 p. 0065	70.00						25		

• 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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Proper	0510 Density at RT (0	Common)		C	Execute Ver	rify Result		
Analys	is Condition		- Select Con	nnonents	\sim			
Analysi	s Method : ◯ y=∑a,x,+k		Select	Il Component	Clear All Comp	ment	Apply	
	⊙ v=Σav +a		Joiour P			data	(hhhi)	
	• 1	x x ~ , - [aa]	S Exclud	le component ten	ms less than 3			
variable	ey: ●y ○ 1/y	log y	Excine	ie 2-&3- 🗸 com	iponent terms und	ier t = 0.0 💌		
					Component	Number	Component	
Select	Component	Coefficient	Std. Error	t Value	vs Property	Humber	vs Property	
					Correlation	of Data	Plot	
V	SIO2				-0.37983	470	Figure	-
V	B2O3				0.32153	173	Figure	
2	AI2O3				0.03013	207	Figure	
1	MgO				-0.05656	30	Figure	
×	CaO				-0.07754	123	Figure	
2	BaO				0.18052	73	Figure	
1	Li20				-0.09843	33	Figure	
×	Na2O				-0.27175	177	Figure	
2	к20				-0.20754	142	Figure	
*	MnO				0.05356	5	Figure	
2	CuO				-0.07595	5	Figure	
2	ZnO				0.41719	475	Figure	
*	SrO				0.11720	28	Figure	
×	PbO				0.49581	25	Figure	
2	Fe2O3				-0.04727	25	Figure	
×	As203				-0.00182	43	Figure	
×	Y2O3				0.16244	23	Figure	•

🍅 inte	RGLAD 8 : Execution of Reg	ression Analysis					- 0	×
File To	ools Help							
S 6	9 🗵 ? 🞯 🕼				INTERGLA	0 8: Regres	sion Analy	sis
Proper	ty 0510 Density at RT (Common)			Execute Ver	rify Result)	
Analys	is Condition		Select Com	ponents				
Analysi	s Method : ○ y=∑a _i x _i +i	¢	Select A	Il Component	Clear All Comp	onent	Apply	
	y=Σa _i x _i +a	a _x x _x Σx _i ≥99 v %	Exclud	e component terr	ms less than 3	data		
variable	ey: ● y ○ 1/y	O log y	Exclud	e 2-&3- 🔻 com	ponent terms und	ler t = 0.0 🔻		
Select	Component	Coefficient	Std. Error	t Value	Component vs Property Correlation	Number of Data	Component vs Property Correlation Plot	
V	SIO2	2.26435E00	0.032	70.848	-0.37983	438	Figure	1-
2	B2O3	2.58839E00	0.089	29.204	0.32153	148	Figure	
V	AI2O3	2.66068E00	0.161	16.519	0.03013	190	Figure	
1	MgO	3.29622E00	0.275	11.989	-0.05656	25	Figure	
2	CaO	3.11707E00	0.145	21.545	-0.07754	109	Figure	
V	BaO	6.79839E00	0.150	45.335	0.18052	66	Figure	
2	Li2O	2.43577E00	0.133	18.249	0.09843	33	Figure	
2	Na2O	2.87075E00	0.116	24.774	0.27175	170	Figure	
V	к20	2.60036E00	0.114	22.876	0.20754	137	Figure	
V	MnO	4.81958E00	0.186	25.851	0.05356	5	Figure	
V	CuO	5.27396E00	2.939	1.794	-0.07595	5	Figure	
	ZnO	4.66743E00	0.044	105.598	0.41719	443	Figure	
V	SrO	5.53116E00	0.229	24.131	0.11720	26	Figure	
V	PbO	9.25409E00	0.272	34.037	0.49581	25	Figure	
×.	Fe2O3	3.40323E00	1.418	2.400	-0.04727	20	Figure	
V	As203	-1.06933E01	13.152	-0 613	-0.00182	43	Figure	
×	Y2O3	8.32568500	0.237	35.198	0.16244	23	Figure	-

- Execute the multiple regression analysis at the default setting by clicking the [Execute] button.
- [Question] dialog boxes appear one after one. Check the dialog, and click the [OK] button for them.

QUESTIC	N ×
?	All components of some glasses have the same values. Are the last 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.
QUESTIC	× x
	All selected components of some glasses have the same values. Are the last data used for analysis, and are other glass data not used? 510 GJ07-382495 [except] 511 GJ07-382496

- 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 R² (0.9613) 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. R² value of ≥0.8 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 (1).
- In this example, |t| of CuO, As₂O₃, Sb₂O₃ and Ho₂O₃ are <2. First, delete ✓ in the checkboxes of As₂O₃, Sb₂O₃ and Ho₂O₃ with |t|<1, and recalculate by clicking the [Execute] button. Second, delete ✓ of CuO 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 (0.9068).

- 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/cm³) = $2.266 \times (SiO_2) + 2.587 \times (B_2O_3) + 2.666 \times (Al_2O_3) + \dots$

 $(SiO_2), (B_2O_3), \dots$: mole ratio of each component (27 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 – 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 for the zinc-silicate glass system obtained in Example 7 is used.

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

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	/			-)	Dotail	_							•
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	Tot	al Number	535 Co	om	ponent Unit mol%	 Information 		*,-,*,						
	Nu	mber of Sources	147	Pr	operty Unit Common	· •	C	ompone	nt	Analyz				
Delete	No.	Glass No.	ensity at RT (g/cm3)		Density at RT (Predictive Value)	Density at RT (Residual)	SiO2	B2O3	AI2O3	MgO	CaO	Ва		
	1	GB02-000500	2.	74	2.771	-3.116E-02	65.00						•	
	2	GB02-000501	2.8	67	2.891	-2.43E-02	60.00						=	
	3	GB02-000502	2	99	3.011	-2.143E-02	55.00							
	4	GB02-000503	3.1	15	3.132	-1.657E-02	50.00							
	5	GB02-000504	2.4	05	2.419	-1.411E-02	75.00							
	6	GB02-000505	2	.51	2.539	-2.925E-02	70.00							
	7	GB02-000506	2.6	36	2.659	-2.338E-02	65.00							
	8	GB02-000507	2.8	85	2.9	-1.465E-02	55.00							
	9	GB02-000508	2.4	39	2.427	1.153E-02	70.00							
	10	GB02-000509	2.	55	2.548	2.397E-03	65.00							
	11	GB02-000510	2.	66	2.768	-1.083E-01	50.00							-



- 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 value in the [New] cells of the [Content] column to predict a property. By clicking the [Calculate] button, the calculated value appears in the [Predictive Value] cell of the [Property] column.
- The predicted density: 2.780 g/cm³.

9. Composition optimization - Zinc-silicate glass with a specified density

Obtain a composition of zinc-silicate glass with density of 2.6 g/cm³ at RT. The components of the glass are SiO₂, Al₂O₃, CaO, Na₂O, K₂O and ZnO.

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

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

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

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<u> </u>					\sim				De	etail				
		Total Num	ber	535	Comp	onent Ur	nit mol%	-	Infor	mation +,-	.*.1			
		Number of	Source	es 147	Pro	operty Ur	nit Comr	non 👻		Comp	onent Analyze			
Delete	No.	Glass No.		··· SIO2	AI2O3	CaO	Na2O	К20	ZnO	Density at RT (g/cm3)	Density at RT (Predictive Value)	Densi (Res	ly at RT idual)	
	501	GJ03-381758							_	2.481	0			1
	502	GJ03-381992		64.47	1.46	11.25	11.20	0.05	7.60	2.67	2.852		-8.24E-02	2
	503	GJ07-381993		58.84	1.37	10.32	10.26	0.81	15.55	2.63	2.826		1.964E-01	1
	504	GJ07-381994		52.99	1.22	0.21	0.28	0.76	23.04	2.09	3.009		3.194E-01	1
	505	GJ07-381995		46.67	1.06	8.16	8.14	0.64	32.98	2.75	3.207		4.572E-0	1
	506	GJ07-381996		40.23	0.88	7.04	7.04	0.51	42.39	2.84	3.412		5.719E-0	1
	507	GJ07-382492		49.96					33.99	3.835	3.7		1.348E-0	1
	508	GJ07-382493		49.99					33.99	3.845	3.704		1.412E-0	1
	509	GJ07-382494		50.00					33.99	3.839	3.705		1.34E-0	1
	510	GJ07-382495		50.00					34.00	3.835				
	511	GJ07-382496		50.00					34.00	3.832	3.706		1.256E-0	1
	512	GJ02-382603		68.75	1.00		13.00		12.00	2.854	3.07		2.161E-0	1
	513	GJ07-382604		66.42	0.97		12.55		15.00	3.007	3.115		1.084E-0	1
	514	GJ07-382605		64.07	0.93		12.12		18.00	3.051	3.161		-1.1E-0	1
	515	GJ06-383138		59.86	19.96				9.98	2.73	2.754		2.444E-02	2
	516	GJ07-383155		69.84	14.97				14.97	2.68	2.752		7.203E-02	2
	517	GJ07-383156		59.86	19.96				19.96	2.84	2.892		5.189E-02	2
	518	GJ07-383157		54.88	9.98				34.92	3.24	3.211		2.859E-02	2
	519	GJ07-383158		49.89	9.98				39.91	3.42	3.331		8.87E-0	2
- 1		0.103 000 FD			0.00			-		A. 8A	A 181		2005.0	3







- Open the [Data List for Regression Analysis] window, and by clicking the [Open] icon open that 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. 503(GJ07-381993) with density of 2.83 g/cm³ 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 (minimun 1%), and the difference is magnified for easy visualization.
- Next sort the content values in the [New] column, and correct the values of B2O3, MgO, BaO and Fe3O3, which are not included in the target composition with 6 components, to 0.
- 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, decrease the content of ZnO with a high coefficient little by little.
- In final the Density at RT becomes 2.600 g/cm³ in case of the following composition.

The composition: SiO₂ 67.49 mol%, Al₂O₃ 1.57%, CaO 11.84%, Na₂O 11.77%, K₂O 0.93%, ZnO 6.41%.

• The composition with the target property is not only one. Therfore calculate changing the other components also, and optimize the composition.

10. Composition optimization (Automatic calculation)- Zinc-silicate glass with a specified density

In the same example as 3.3, obtain a composition of zinc-silicate glass with density of 2.6 g/cm³ at RT. The components of the glass are SiO₂, Al₂O₃, CaO, Na₂O, K₂O and ZnO.

<Refer to D.4 of Chapter 3, and 4.8, 4.9 of Chapter 4>
Composition optimization is performed by the least squares method using a new multiple regression equation from the search result in Example 7.

1) Search result ([Data List for Regression Analysis] window) \rightarrow Selection of explanatory variables ([Select Component Terms] dialog boxes)

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Delete	No.	Glass No.	Data	a Source	Year	Data S Num	ource Iber	Density a (g/cm)	tRT 3)	Densi (Predict	ty at RT ive Value)	Den: (Re	iity at RT sidual)
	501	GJ03-381758	J. Americ	an Cerami	2015	v. 098 p. 07	48		2.481				^
	502	GJ03-381992	J. Mater.	Sci.: Materi	2017	v. 028 p. 40	64		2.57				
	503	GJ07-381993	J. Mater.	Sci.: Materi	2017	v. 028 p. 40	64		2.63				
	504	GJ07-381994	J. Mater.	Sci.: Materi	2017	v. 028 p. 40	64		2.69				
	505	GJ07-381995	J. Mater.	Sci.: Materi	2017	v. 028 p. 40	64		2.75				
	506	GJ07-381996	J. Mater.	Sci.: Materi	2017	v. 028 p. 40	64		2.84				
	507	GJ07-382492	J. Materia	als Science	2018	v. 053 p. 01	1204		3.835				
	508	GJ07-382493	J. Materia	als Science	2018	v. 053 p. 01	1204		3.845				
	509	GJ07-382494	J. Materia	als Science	2018	v. 053 p. 01	1204		3.839				
	510	GJ07-382495	J. Materia	als Science	2018	v. 053 p. 01	1204		3.835				
	511	GJ07-382496	J. Materia	als Science	2018	v. 053 p. 01	1204		3.832				
	512	GJ02-382603	Ceramic	s - Silikaty	2018	v. 062 p. 01	88		2.854				
	513	GJ07-382604	Ceramic	s - Silikaty	2018	v. 062 p. 01	88		3.007				
	514	GJ07-382605	Ceramic	s - Silikaty	2018	v. 062 p. 01	88		3.051				
	515	GJ06-383138	J. Non-C	rystalline S	2018	v. 502 p. 01	90		2.73				
	516	GJ07-383155	J. Non-C	rystalline S	2018	v. 502 p. 01	90		2.68				
	517	GJ07-383156	J. Non-C	rystalline S	2018	v. 502 p. 01	90		2.84				_
	518	GJ07-383157	J. Non-C	rystalline S	2018	v. 502 p. 01	90		3.24				E
	519	GJ07-383158	J. Non-C	rystalline S	2018	v. 502 p. 01	90		3.42				-
		0.000.000.000	1		00.00	600 04			0.50				

- Open the [Selection of 1 Component Terms] dialog box by clicking the [Component] button, and specify component terms for a multiple regression equation.
- In this example, first click the [Clear All Component] button in the [Select Component Terms] dialog box for the Selection of 1-Component Terms, and check the 6 checkboxes of SiO₂, Al₂O₃, CaO, Na₂O, K₂O and ZnO. Click the [OK] button.
- Check the number of the component terms in the [Question] dialog box.

1-Component Terms: 6.

• Click the [Analyze] button.

🍅 Se	elect Component Ten	ms		×
	Selectiion of 1-Con If necessary, cha Min. num. of gla Min. num. of gla Select All Co	ange the following con sses = 1 % of sses = 2 glas omponent Clear	dition : Apply total retrived glasse ses to one compone All Component	ent
\wedge	Component	Number of Glasses	Max. Content %	
	SiO2	470	85.000	-
	B2O3	173	50.000	
V	AI2O3	207	25.000	
	MgO	30	30.000	=
V	CaO	123	38.200	
	BaO	73	30.000	– µ
	Li2O	33	35.000	
V	Na2O	177	40.000	
V	K20	142	35.000	
	MnO	5	45.000	
	FeO	1	0.540	
	C00	2	1.790	
	CuO	5	3.140	
	ZnO	475	70.000	
	SrO	28	30.000	
	CdO	1	40.000	
	PbO	25	40.000	
	SnO	0	0.000	-
	BACK	Next OK	Cancel	



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

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Proper	ty 0510 Density at RT (0	Common)		Б	kecute Veri	fy Result		
Analys	is Condition		Select Com	ponents				
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	⊛ y=Σa,x,+a	xx Σx 299 -	% 🗹 Exclud	e component terr	ns less than 3	data		
variabl	ey: 🖲 y 🔾 1/y	🔾 log y	Exclud	e 2-&3- 🔻 com	ponent terms und	ier t = 0.0 🔻		
Select	Component	Coefficient	Std. Error	t Value	Component vs Property Correlation	Number of Data	Compo vs Pro Correl Plo	nent perty ation ot
V	SiO2	2.27863E00	0.034	66.480	-0.37983	439	Figu	re
r	AI2O3	2.88409E00	0.158	18.284	0.03013	190	Figu	re
r	CaO	3.37441E00	0.167	20.253	-0.07754	109	Figu	re
r	Na2O	2.85652E00	0.106	27.034	-0.27175	170	Figu	re
r	К2О	2.55682E00	0.098	26.132	-0.20754	137	Figu	re
r	ZnO	4.69083E00	0.061	77.060	0.41719	444	Figu	re
	lv.	7.07604500	4 070	1.605			Figu	ro

- Execute the multiple regression analysis with the 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. Confirm R²=0.9091 and t value≥18.3.

3) Composition optimization by automatic calculation

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Delete	No	. Glass No.				SiO2	AI2O3	Ca	Na2O	К20	ZnO	Densit	(atRT m3)	Densi (Predicti	ty at RT ve Value)	Der (R	nsity at RT esidual)	ſ
	10	GB02-000509				65.00					10.00		2.55					7
	11	GB02-000510				50.00					18.75		2.66					
	12	GB02-000511				65.00					5.00		2.47					
	13	GB02-000512				60.00					10.00		2.574					
	14	GB02-000513				55.00					15.00		2.675					
	15	GB02-000514				60.00					5.00		2.49					
	16	GB02-000515				55.00					10.00		2.597					
	17	GB02-000516				50.00					15.00		2.705					
	18	GB02-000758				50.00			15.00)	35.00		3.215		3.21		5.418E-0	13
	19	GB02-000759				50.00			20.00)	30.00		3.091		3.118		-2.687E-0	2
	20	GB02-000760				50.00			25.00)	25.00		2.979		3.026		-4.715E-0	12
	21	GB02-000761				50.00			30.00		20.00		2.87		2.934		-6.444E-0	2
	22	GB02-000762				50.00			35.00)	15.00		2.776		2.843		-6.672E-0	2
	23	GB02-000763				50.00			40.00)	10.00		2.851		2.751		9.999E-0	12
	24	GB02-000764				60.00			10.00)	30.00		3.173		3.06		1.129E-0	1
	25	GB02-000765				60.00			15.00)	25.00		3.057		2.968		8.864E-0	2
	26	GB02-000766				60.00			20.00)	20.00		2.93		2.877		5.335E-0	2
	27	GB02-000767				60.00			25.00)	15.00		2.818		2.785		3.307E-0	2
	28	GB02-000768				60.00			30.00)	10.00		2.717		2.693		2.378E-0	2
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• Go back to the [Data List for Regression [Analysis] window, and by clicking the [LSM] icon open the [Composition Optimization (LSM)] window.



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?	Do you set the initial value of a component that is not an explanatory variable of multiple regression equation to 0? Component values that are not explanatory variables of multiple regression equations are fixed.

- Input the target value in the [Target] column (in this example, Density at RT=2.6 g/cm³).
- Click the [All Calc (LSM)] button. The [Question] dialog box, 'Do you set the initial value of a component that is not an explanatory variable of multiple regression equation to 0?' opens, and click the [OK] button.

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	Glass No	Density at RU	Density at RT (R	•	All Prop (Res.)	5	SiO2	AI203	CaO	Na2O	K20	ZnO	Г
265	GB07-174630	2.6004	1.55821E-4	A	1.55821E-4	A	73.613	0.0	0.0	17.157	0.0	9.22923	ŀ
29	6B02-000769	2.6015	5.77309E-4	A	5.77309E-4	A	60 6	0.0	0.0	35.0	0.0	5.0	F
183	GB02-096226	2.59825	6.7398E-4	А	6.7398E-4	A	69.5825	0.0125	0.00704	22.511	0.02922	7.84736	
186	GB02-096229	2.59809	7.34616E-4	A	7.34616E-4	A	74 859	0.02652	0.02026	16.238	0.01936	9.33514	
184	GB02-096227	2.59802	7.609E-4	A	7.609E-4	A	71.005	0.00582	0.01654	20.678	0.01837	8.27574	
111	GB02-016306	2.59796	7.86126E-4	A	7.86126E-4	A	9.010	0.01562	0.00976	23.309	0.00975	7.64422	
55	GB02-000940	2.60206	7.906E-4	A	7.906E-4	A	60.311	4.99835	4.99658	0.01077	22.383	7.29972	4
388	GJ02-359367	2.60208	8.00263E-4	A	8.00263E-4	A	64.580	6.11763	6.11404	11.339	6.18153	5.66649	4
26	GB02-000766	2.60211	8.1192E-4	A	8.1192E-4	A	72.702	5.11554	5.73833	2.45402	5.71759	8.27228	
57	GB02-000942	2.60214	8.22174E-4	A	8.22174E-4	A	55.143	5.00078	4.99807	0.01039	28.2179	6.62901	
393	GJ07-359372	2.60216	8.31445E-4	A	8.31445E-4	A	74.196	5.00556	5.29956	0.00834	6.49252	8.99785	
173	GJ02-071993	2.59781	8.40768E-4	A	8.40768E-4	A	63.798	0.00773	0.00836	30.172	0.01733	5.99592	
59	GB02-000944	2.60219	8.40915E-4	A	8.40915E-4	A	37.842	4.9889	5.00703	0.0028	47.783	4.375	
121	GB07-022502	2.60219	8.4273E-4	A	8.4273E-4	A	62 107	23.863	4.99731	1.0E-5	4.38325	4.64816	
67	GB02-000952	2.59781	8.44044E-4	A	8.44044E-4	A	65.710	0.00905	0.00959	4.99194	19.497	9.79068	
77	GB02-000962	2.60221	8.48938E-4	А	8.48938E-4	A	43.158	5.57704	5.57704	0.0	40.926	4 6115	
60	GB02-000945	2.5977	8.49496E-4	A	8.49496E-4	A	69.684	0.00971	0.01948	4.97779	15.012.	10.296	
227	GB02-138958	2.597/9	8.50168E-4	A	8.50168E-4	A	66.818	0.04827	0.0093	2.26455	20.588	10.301	

- After calculation, the [Result of Composition Optimization (LSM)] window opens. In the table, sort the [All Prop (Res.)] values in ascending order by clicking the title column, All Prop (Res.). In this example 153 glasses with density values lower than 0.1% to the target value are obtained. They are marked as A and their background color of Glass No. is blue. Each composition is indicated in the component columns in the right-hand side of the table.
- One of examples of composition optimized is as follows. In case of No. 388 (The model glass, GJ02-359367), SiO₂ 64.58 mol%, Al₂O₃ 6.12%, CaO 6.11%, Na₂O 11.34%, K₂O 6.18% and ZnO 5.67%. Its density at RT is 2.602 g/cm³.
- The user can use also the multiple regression equation obtained in Example 7. for automatic calculation. In

this case, compositions with 27 components as the explanatory variables are obtained.

11. Property prediction by a linear equation — Young's modulus of alkaline-earth silicate glasses Predict Young's modulus at RT of an alkaline-earth silicate glass 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) \rightarrow Search



- Specify 20≤SiO₂≤80 mol% for the Composition. Select 'Alkaline-earth Silicate' for the Glass System, '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) \rightarrow Selection of explanatory variables ([Selection of 1, 2, 3-Component Terms] dialog boxes)

🔯 INTE	RGLAD	8 : Data List for Reg	pression A	nalysis						- () X
File To	ols He	alp									
-	a 🗆		2 L	12 to t	9 C.9		2	🙆 🙆 D		Pegression A	nalveie
	- J -		ग्टर्ज (गटर्ज)	- mai a	जर्म । दास	19221 19221		• [•] I	TERGLAD 0.	Regression	indiysis
								Detail			
		otal Number	573	ompon	ent Un	it mol%	Ţ	Informatio	on +*./		
	~						-				
	N	umber of Source	s 96	Prope	rty Un	t Common			Component	Analyze	
Delete	No.	Glass No.	Dat	a Source	Year	Data S Num	ource iber	SiO2	Young's Modulus at (GPa)	Young's Modulus at (Predictive Value)	Young's (Re
	1	GJ02-003209	J. Ceram	nic Soc. Ja	1988	v. 096 p. 10	12	30.00	1.067E+02		^
	2	GJ03-003210	J. Ceram	nic Soc. Ja	1988	v. 096 p. 10	12	30.00	1.032E+02		Ξ
	3	GB02-006471	Handbo	ok of Glass	1986	v. 001 p. 03	326	58.80	6.03E+01		
	4	GB02-006474	Handbo	ok of Glass	1986	v. 001 p. 03	326	52.30	6.59E+01		
	5	GB02-006477	Handbo	ok of Glass	1986	v. 001 p. 03	326	59.00	6.21E+01		
	6	GB02-006479	Handbo	ok of Glass	1986	v. 001 p. 03	326	55.80	6.68E+01		
	7	GB02-006480	Handbo	ok of Glass	1986	v. 001 p. 03	326	53.20	6.83E+01		
	8	GB02-006485	Handbo	ok of Glass	1986	v. 001 p. 03	326	59.60	6.86E+01		
	9	GB02-006487	Handbo	ok of Glass	1986	v. 001 p. 03	326	56.60	7.0E+01		
	10	GB03-006508	Handbo	ok of Glass	1986	v. 001 p. 03	36	50.00	8.1E+01		
	11	GB03-006509	Handbo	ok of Glass	1986	v. 001 p. 03	36	50.00	8.25E+01		
	12	GB03-006510	Handbo	ok of Glass	1986	v. 001 p. 03	36	50.00	8.28E+01		
	13	GB03-006511	Handbo	ok of Glass	1986	v. 001 p. 03	36	50.00	8.4E+01		
	14	GB03-006512	Handbo	ok of Glass	1986	v. 001 p. 03	36	50.00	8.36E+01		
	15	GB03-006513	Handbo	ok of Glass	1986	v. 001 p. 03	36	55.00	8.03E+01		4
	16	GB03-006514	Handbo	ok of Glass	1986	v. 001 p. 03	36	55.00	8.16E+01		
	17	GB03-006515	Handbo	ok of Glass	1986	v. 001 p. 03	36	55.00	8.22E+01		
	18	GB03-006516	Handbo	ok of Glass	1986	v. 001 p. 03	36	55.00	8.32E+01		
	19	GB03-006517	Handbo	ok of Glass	1986	v. 001 p. 03	36	55.00	7.81E+01		
_	~~	0000000000	4						0.005.04		
_			1.1				_				

QUESTION	\times
Suberton of EXplanetory Variables in Multiple Regression Anal 1.Component Terms: 0 3.Component Terms: 0 0K Cancel	ysis:

- 573 glasses are listed.
- After clicking the [Component] button, specify only 1component terms for explanatory variables at the default setting.

1-componet terms: 27.

ſ	Selectiion of 1-Con	nponent Terms		٦
	If necessary, chi	ange the following cor	dition : Apply	L
	Min. num. of gla	sses = 1 % o	f total retrived glasses	I.
	Min. num. of gla	sses = 2 glas	ses to one componen	t
				1
	Select All Co	omponent	All Component	
	Component	Number of Glasses	Max. Content %	
*	SIO2	573	60.000	
*	B2O3	70	35.000	
*	AI2O3	424	36.100	
2	MgO	325	46.150	
*	CaO	333	55.000	
*	BaO	81	45.000	
*	Li2O	50	24.400	
*	Na2O	204	31.500	
*	K20	89	24.400	
*	BeO	55	39.700	
	MnO	1	3.050	
	FeO	1	0.130	
*	ZnO	15	33.330	
2	SrO	80	45.000	
2	CdO	5	33.330	
	PbO	3	0.600	
	Cr2O3	1	0.004	
2	Fe2O3	15	4.900	
	·			

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

🝅 inte	RGLAD 8 : Execution of Reg	ression Analysis					- 0	×
File To	ools Help							
S 6	3 🗵 ? 😝 😒				INTERGLAD	8: Regres	sion Analy	sis
Proper	ty							
0	540 Young's Modulus at I	RT (Common)			xecute	ity Result		
Analys	is Condition		Select Compo	onents				
Analysi	sMethod: ○ y=Σa _i x _i +l	¢ (Select All C	Component	Clear All Compo	onent	Apply	
	(a) y=Σa,x,+a	a_x_ Σx, 2 99 🔟 🐝	Exclude o	omponent terr	ns less than 3	data		
			✓ Exclude	2-83- 🔻 com	ponent terms und	ler Itl= 0.0 💌		
variable	ey: ⊚y ⊖ 1/y	⊖ log y						
			\frown		Component	Number	Component	
Select	Component	Coefficient	Std. Error	t Volue	vs Property		Correlation	
					Correlation	of Data	Plot	
×	SiO2	7.04206E01	2.518	27.97	-0.53734	516	Figure	
×.	B203	9.74954E01	7.235	13.476	-0.19922	70	Figure	
×	AI203	1.27794E02	4.534	28.184	0.31651	398	Figure	
×	MgO	1.50469E02	3.899	38.589	0.66954	304	Figure	
×	CaO	1.11249E02	3.707	30.013	-0.03850	312	Figure	
×	BaO	6.80630E01	5.848	11.639	-0.27821	73	Figure	
2	Li2O	1.50233E02	11.932	12.591	0.05758	50	Figure	
×	Na2O	2.80877E01	7.323	3.835	-0.53609	192	Figure	41
V	к20	2.61444E01	9.681	2.701	-0.36504	82	Figure	
V	BeO	2.07404E02	5.202	39.870	0.49875	47	Figure	40
×	ZnO	1.09489E02	15.617	7.011	-0.09067	15	Figure	
	SrO	8.76814E01	5.484	15.990	-0.22006	66	Figure	
	CdO	8.32692E01	17.395	4.787	-0.09318	3	Figure	
	Fe2O3	-4.75316E02	56.552	-8.405	-0.18667	15	Figure	
	AS203	1.49198E01	1427.956	-0010	-0.12060	16	Figure	
	Y2O3	2.94557E02	19.288	15.271	0.29927	42	Figure	
	La203	-9.25125E01	1/5.050	-0.528	-0.05015	6	Figure	-

• By clicking the [Analyze] button, the [Execution of Regression Analysis] window opens. Click the [Execute] button, and click the [OK] button in each [Question] dialog box which appears one after another. Finally the regression coefficients, etc. are shown.



iNTERGLAD 8 : Execution of Regre

Analysis Method : $\bigcirc y = \sum a_i x_i + k$

Property 0540 Young's Modulus at RT (Common)

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Analysis Co

ariable

Select

✓ SrO

-P205

N

Nd2O3 TiO2 ZrO2 SnO2

BaCl2 N AIN SIC Si3N4

on Analysi

• $y = \sum a_i x_i + a_x x_x \sum x_i \ge gg \checkmark g_g$ ● y ○ 1/y ○ log y

Coefficient

9.42283E01 8.04829E01

-4.61331E0

3.06915E02

2.51317E02

1.47284E02

2.22362E02 -3.33742E03

9.82670E01

4.18528E0 2.50889E0 1.48839E0

4.95383E02

-4.81299E0

Std. Error

70.430

6.946

18.103 1292.065

14.949

26.052 11.759 32.333

48.296

346.422

3.568

21.204

12.283

6.574

16.065 21.336 4.603

10.25

0.07490

0.13222

0.23143

-0.18592

-0.06350

0.19848 0.17220

0.0293

0.15111

Open the [Verification of Regression analysis]
window by clicking the $\left[\text{Verify Result} \right]$ button. The
contribution rate $R^{\scriptscriptstyle 2}$ is 0.8826. 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 deletion.

			D 8: Regres	sion Analys	is
Select Com Select Al	nponents Il Component	Clear All Comp	onent	Apply	
Exclude	e component terr e 2-&3- 💌 com	ns less than 3 ponent terms un	data der t = 0.0 💌		
Std. Error	t Value	Component vs Property Correlation	Number of Data	Component vs Property Correlation Plot	
4.316	21.831	-0.22006	66	Figure	<u> </u>
13.349	6.029	-0.09318	3	Figure	
43.723	-10.551	-0.18667	15	Figure	
		-0.12060	16	Figure	
14.831	20.694	0.29927	42	Figure	
		-0.05015	6	Figure	

×

Figure

nd P₂O₅ are <2. Delete ✓ ick the [Execute] button



- In this case \mathbb{R}^2 is 0.9265 (≥ 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 mol%, Al_2O_3 12%, MgO 13%, CaO 20%, Y_2O_3 7%, TiO₂ 3%) in the [New] cells, and click the [Calculate] button.

• 114.1 GPa for Young's modulus appears in the [Predictive Value] cell of the [Property] column.

12. Property prediction by a cubic equation - Density of boro-silicate glasses

Predict density at RT of a glass of SiO₂-B₂O₃-K₂O system with the following composition. SiO₂ 40%, B₂O₃ 30%, K₂O 26%, CaO 3%, Al₂O₃ 1% (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) \rightarrow Search



- Specify the following condition of composition. SiO_2 + $B_2O_3 + K_2O \geq 95 \mbox{ mol}\%$
- Select 'Density at RT' for the Property and 'NOT Patent' for the Data Source.

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

4	* 🖬			흹뎚		6 6 IN	TER	SLAD	8: Regression	Analysi
		~	-			Detail				
		otal Number	351 Compor	ent Un	t mol% 💌	Informatio	m	A		<u> </u>
	V	umber of Source	es 47 Prop	erty Un	t Common 👻			Compon	ent Analyze)
Delete	No.	Glass No.	Data Source	Year	Data Source Number	SiO2	B203	K20	Density at R1 (g/cm3)	Density : (Predictive
	1	G805-001398	Handbook of Glass	1986	v. 001 p. 0084	15.00	55.00	30.00	2.448	
	2	G802-001399	Handbook of Glass.	1986	v. 001 p. 0084	68.00	4.00	28.00	2.458	
	3	G802-001400	Handbook of Glass	1986	v. 001 p. 0084	68.00	8.00	24.00	2.459	
	4	G805-001401	Handbook of Glass	1985	v. 001 p. 0084	15.00	65.00	20,00	2.223	
	5	G802-001402	Handbook of Glass	1986	v. 001 p. 0084	65.00	15.00	20.00	2.468	
	6	G805-001403	Handbook of Glass.	1986	v. 001 p. 0084	52.00	32.00	16.00	2.387	
	7	G805-001404	Handbook of Glass.	1986	v. 001 p. 0084	60.00	24.00	16.00	2.444	
	8	G805-001405	Handbook of Glass	1986	v. 001 p. 0084	64.00	20.00	16.00	2.463	
	9	GB05-001406	Handbook of Glass.	1985	v. 001 p. 0084	68.00	16.00	16.00	2.477	
	10	GB02-001407	Handbook of Glass	1986	v. 001 p. 0084	72.00	12.00	16.00	2.473	
	11	G802-001408	Handbook of Glass.	1985	v. 001 p. 0084	76.00	8.00	16.00	2.445	
	12	G802-001409	Handbook of Glass	1986	v. 001 p. 0084	80.00	4.00	16.00	2.403	
	13	G805-001410	Handbook of Glass	1986	v. 001 p. 0084	15.00	70.50	14.50	2.083	
	14	G805-001411	Handbook of Glass	1986	v. 001 p. 0084	15.00	75.00	10.00	2.014	
	15	G805-001412	Handbook of Glass	1986	v. 001 p. 0084	68.00	24.00	8.00	2.217	
	16	G805-001413	Handbook of Glass	1986	v. 001 p. 0084	65.00	30.00	5.00	2.13	
1	17	G805-001414	Handbook of Glass	1986	v. 001 p. 0084	68.00	28.00	4.00	2.121	
	18	G805-001415	Handbook of Glass	1985	v. 001 p. 0084	15.00	82.00	3.00	1.842	
				1						

3) Regression analysis by a linear equation

	If necessary, change the following condition : Apply											
	Min. num. of glasses = 1 % of total retrived glasses											
Min. num. of glasses = 2 glasses to one component												
Select All Component Clear All Component												
	Component	Number of Glasses	Max Content %									
V	SiO2	351	97.210									
V	B2O3	351	82.000									
V	К20	351	62.500									
V	AI2O3	28	3.190									
	MgO	1	0.310									
V	CaO	9	3.390									
	BaO	2	1.280									
V	Li2O	13	4.500									
V	Na2O	68	5.000									
	FeO	1	0.160									
V	ZnO	3	1.870									
	PbO	1	0.110									
	Fe2O3	1	0.004									
V	As2O3	10	0.550									
	Sb2O3	2	0.090									
	TiO2	1	0.020									
	он	2	0.140									
~	U02	4	0.500									

• First, regression analysis by a linear equation is carried out for comparison.

• After clicking the [Component] button, specify only 1component terms for explanatory variables at the default setting.

10 component terms for 1-componet terms are selected.



rs1 ∉	3 📝 🦻 👩 🚳			IN	TERGLAD	3: Regressi	on Analys
Proper	ty				\sim		
	0510 Density at RT (Common)		E	kecute Veril	ly Result	
Analys	is Condition		Select Com	ponents			
Analysis Method : ○ y=∑a,x,+k			Select Al	Il Component	Clear All Compo	onent	Apply
	y=Σa.x.+a	x Σx.299 -	Exclude	e component terr	ns less than 3	data	
	© · · · ·	** !	Exclude	2.83 T com	nonent terms und	ler Iti= 0.0 💌	
variable	ey: ●y ◯ 1/y	o log y	E EXCIUD		ponent termo une		
					Component	Number	Component
Select	Component	Coefficient	Std. Error	t Value	vs Property		VS Property Correlation
					Correlation	of Data	Plot
¥	SIO2	2.42180E00	0.014	171.814	0.22752	276	Figure
	B2O3	1.97499E00	0.024	81.004	-0.57124	276	Figure
×	к20	2.81713E00	0.039	72.181	0.47269	276	Figure
×	AJ2O3	-1.22568E-01	1.601	-0.077	-0.17345	27	Figure
~	CaO	1.76864E00	2.252	0.785	-0.02108	9	Figure
2	Li2O	-1.31340E00	1.105	-1.188	-0.19504	13	Figure
*	Na2O	1.84135E00	0.383	4.814	-0.12867	64	Figure
×	ZnO	6.47575E00	4.250	1.524	0.02616	3	Figure
K	As2O3	-4.91010E00	12.073	-0.407	-0.05368	10	Figure
~	U02	3.04447E01	15.747	1.933	0.07717	4	Figure
	Xx	-1.99327E01	13.317	-1.497			Figure

• By clicking the [Analyze] button, the [Execution of Regression Analysis] window opens. Click the [Execute] button and the [Verify Result] button. The contribution rate R^2 is relatively low, 0.5806.



4) Regression analysis by a cubic equation



🖌 😓 Se	lect Component Terr	ns					2	×	
Select	tion of 2-Componer	it Term	1S —						
1 E	If necessary, cha	inge th	e follo	wing c	ondi	ition : Apply			
🗹 Mir	n. num. of glasses :	-	7 % of total retrieved gla						
Mir	n. num. of glasses :	-	10	onent					
🖌 Ma	x. num. of compon	ents =	50	%	of n	um. of 1-compo	nent terr	ns	
s	Select All Co	mpon	ent	Cle	ar A	II Component			
	Component	Num	ber of	Glasse	s I	Max. Content %			
V	SiO2			3	51	97.210		^	
~	B2O3	351				82.000			
V	K20	351				62.500			
2	AI2O3			28	3.190				
	MgO				1	0.310			
	CaO				9	3.390)		
	BaO				2	1.280			
	Li2O				13	4.500			
V	Na2O				68	5.000			
	FeO				1	0.160			
	ZnO				3	1.870			
	PbO				1	0.110			
	Fe2O3				1	0.004			
	As2O3				10	0.550			
	Sb2O3	2			2	0.090			
	TiO2	1			1	0.020			
	он				2	0.140			
	U02				4	0.500		Ŧ	
	BACK	Nex	i	ок		Cancel			

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

Select	tion of 3-Componer	it Terms ——	wing con	dition : Apply					
🖌 Mir	n. num. of glasses :	= 15	15 % of total retrieved glasse						
Mir	n. num. of glasses :	= 10	alas	ses to one compo	nent				
Ma	x, num, of compon	ents = 30	- % of	num, of 1-compor	nent terms				
	Select All Co	omponent	Clear	All Component]				
	Component	Number of	Glasses	Max. Content %					
V	SiO2		351	97.210	-				
V	B2O3		351	82.000					
r	К2О		351	62.500					
	AI2O3		28	3.190					
	MgO		1	0.310					
	CaO		9	3.390					
	BaO		2	1.280					
	Li2O		13	4.500					
	Na2O		68	5.000					
	FeO		1	0.160					
	ZnO		3	1.870					
	PbO		1	0.110					
	Fe2O3		1	0.004					
	As2O3		10	0.550					
	Sb2O3		2	0.090					
	TiO2		1	0.020					
	он		2	0.140					
	U02		4	0.500	-				
	BACK	Next	ок	Cancel					

QUESTION	×
Selection of Explanatory Variables in Multip Scomponent Terms: 10 Scomponent Terms: 1 OK Cancel	le Regression Analysis:

🍅 INTE	RGLAD 8: Execution of Reg	ression Analysis						-		×
File To	ools Help									
B 6	9 🗹 🕐 🥑					INTERGLA	D 8: Regres	sior	Ana	lysis
Proper	ty 0510 C	lensity at RT (Com	mon)			Execute	Verify Result	>		
Analys	is Condition			Select Compone	nts					
Analysi	is Method : $\bigcirc y = \sum a_i x_i + \sum a_i x_i $	ΣΣb _{ij} x _i x _j +ΣΣΣ	ijk X,X,X,+k		Select All Corr	ponent Cle	ar All Component		A	vlag
	(a) y=Σa,x,+2	ΣΣb,,x,x,*ΣΣΣ(x, 2 99 🕶 %	Exclude com	ponent terms les	ss than 3	data	_	
variable	ey: ● y ○ 1/y	log y			Exclude 2-8	3. T compone	nt terms under t =	0.0	-	
Select	Component	Coefficient	Std. Error	talue	Component vs Property Correlation	Number of Data	Component vs Property Correlation Plot			
	SiO2	2.33276E00	0.027	86.349	0.21148	276	Figure			-
*	B2O3	1.69433E00	0.049	34.639	-0.54966	276	Figure			
*	к20	1.40634E00	0.082	17.208	0.44020	276	Figure			
*	AI2O3	5.44621E02	196.811	2.767	-0.19753	27	Figure			
*	CaO	3.15990E00	1.285	2.458	-0.02668	9	Figure			
	LI20	1.63100E00	0.658	2.477	-0.23199	13	Figure			
*	Na2O	9.06973E00	18.585	0.488	-0.10844	64	Figure			
*	ZnO	2.37599E00	3.324	0.715	0.02920	3	Figure			
	As2O3	3.03789E00	6.524	0.466	-0.06520	10	Figure			
*	U02	2.63662E01	8.443	3.123	0.08926	4	Figure			
*	SiO2*B2O3	-1.37953E-01	0.177	-0.781	-0.36814	276	Figure			
*	SiO2*K2O	2.09587E00	0.221	9.476	0.77970	276	Figure			
*	SiO2*Al2O3	-5.77188E02	207.553	-2.781	-0.19892	27	Figure			
*	SiO2*Na2O	-3.36907E00	19.525	-0.173	-0.12000	64	Figure			
	B2O3*K2O	2.78566E00	0.298	9.349	-0.05897	276	Figure			
*	B203*AI203	-5.13687E02	183.879	-2.794	-0.21751	27	Figure			
*	B203*Na20	-1.49483E01	19.415	-0.770	-0.16654	64	Figure			





- Execute the regression analysis in the [Execution of Regression Analysis] window, and open the [Verification of Regression Analysis] window. R² is found to be 0.8848, a good result.
- Check t values in the [Execution of Regression Analysis] window. Component terms with |t|<1 are 7 (1-component 1terms: 3, 2-component terms: 4, 3component terms: 0).
- In the third row of the [Select Components] column in the [Regression Analysis] window, 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 'all' component terms under |t| = '1.0.'
 - 3) Exclude 'all' component terms under
 - |t|='1.0' again.

Finally all the |t| values become ≥ 1.0 , and R²=0.8759. A cubic multiple regression equation is complete.

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.
- Input component values (SiO₂ 40 mol%, B₂O₃ 30%, K₂O 26%, CaO 3%, Al₂O₃ 1%) in the [New] cells of the [Regression Equation/ Content] column, and click the [Calculate] button.
- 2.771 g/cm³ for the calculated density appears in the [Predictive Value] cell of the [Property] column.

Search and Analysis of Structure Data

13. Investigation of correlation between composition and structure – Bridging oxygen fraction vs. SiO_2 content

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

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



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

-	2	B B		INTERG	LAD 8: Glass	Structure			
	(lata Source List				Detail	Information	Compone	nt
Total Number 159 Component Unit mol%						Delete	**.J	Property	y
Number of Sources 15					Undo		Structure	0	
Delete	No.	Glass No.	Data Source	Year	Data Source Number	BO / total O (B-O-B) (%)	BO / total O (B-O-Si) (%)	BO / total O (AI-O-AI) (%)	BO / to (AI-O (%
	1	S-00503	Physics and Chemi	1990	v. 031 p. 0030				-
	2	S-00504	Physics and Chemi	1990	v. 031 p. 0030				
	3	S-00505	Physics and Chemi	1990	v. 031 p. 0030				
	4	S-00506	Physics and Chemi	1990	v. 031 p. 0030				
	5	S-00507	Physics and Chemi	1990	v. 031 p. 0030				
	6	S-00549	J. Chemical Soc. Ja.	1981	v. 089 p. 0599				
	7	S-00550	J. Chemical Soc. Ja.	1981	v. 089 p. 0599				
	8	S-00552	J. Chemical Soc. Ja	1981	v. 089 p. 0599				
	9	S-00553	J. Chemical Soc. Ja.	1981	v. 089 p. 0599				
	10	S-00554	J. Chemical Soc. Ja	1981	v. 089 p. 0599				
	11	S-00555	J. Chemical Soc. Ja.	1981	v. 089 p. 0599				
	12	S-00556	J. Chemical Soc. Ja.	1981	v. 089 p. 0599				
	13	S-00557	J. Chemical Soc. Ja.	1981	v. 089 p. 0599				
	14	S-00558	J. Chemical Soc. Ja.	1981	v. 089 p. 0599				
	15	S-00559	J. Chemical Soc. Ja.	1981	v. 089 p. 0599				
	16	S-00560	J. Chemical Soc. Ja.	1981	v. 089 p. 0599				
	17	S-00561	J. Chemical Soc. Ja.	1981	v. 089 p. 0599				
	18	S-00754	Fall Meeting Ceram	1993	v. 001 p. 0078				
	19	S-00756	Fall Meeting Ceram	1993	v. 001 p. 0078			1.38E+01	

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



• 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 bonding with Si to the total oxygen.

- 159 glasses of 15 data sources are listed.
- BO/[totalO] data of not only Si-O-Si but also Al-O-Al, Si-O-B, Si-O-Al etc. appear in the list.

- An XY plot of SiO₂ content vs. BO/[total O] (Si-O-Si) is shown. In this example, the linear equation is selected as a fitting curve.
- In this example, as composition is not specified in the search condition, various components are contained. It is found that the bridging oxygen (Si-O-Si) increases with increasing SiO₂ content.

14. Investigation of correlation between structure factors — Q² vs. 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) \rightarrow Search



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

🏷 INT	ERGLAD	8 : Data List of St	ructure						- 0	\times	
File T	ools He	alp									
*	2	586	₩ ₩ ₩ (1 🕐 😝 😫		INT	TERGLAD	8: Glass Stru	cture	•
Data Source List						Detail	Inform	nation	Component	ŕ	ĥ
Total Number 42 Compone			nent U	nit mol% 💌	Delete	+, -		Property			
Number of Sources 9						Undo			Structure		
Delete	No.	Glass No.	Data Source	Year	Data Source Number	Glass No (Property)	NBO / total O (0) (%)	NBO / total O (Si-O) (%)	Q2 / total X (Si) (%)		
	1	S-00119	J. Non-Crystalline S.	2002	v. 297 p. 0220	GJ02-219523	2.86E+01		1.0E+	01 📥	
	2	S-00120	J. Non-Crystalline S.	2002	v. 297 p. 0220	GJ02-219524	4.01E+01		2.3E+	01	
	3	S-00121	J. Non-Crystalline S.	2002	v. 297 p. 0220	GJ02-219525	5.49E+01		3.6E+	01	
	4	S-00122	J. Non-Crystalline S.	2002	v. 297 p. 0220	GJ02-219526	2.86E+01		1.0E+	01	
	5	S-00123	J. Non-Crystalline S.	2002	v. 297 p. 0220	GJ02-219527	2.86E+01		1.0E+	01	1
	6	S-00662	J. Materials Science	1993	v. 028 p. 3473	GJ02-141512	8.22E+01		1	9.3	
	7	S-00663	J. Materials Science	1993	v. 028 p. 3473	GJ02-141513	8.23E+01		3.05E+	01	
	8	S-00664	J. Materials Science	1993	v. 028 p. 3473	GJ02-141514	7.03E+01		6.06E+	01	
	9	S-00665	J. Materials Science	1993	v. 028 p. 3473	GJ02-141515	5.11E+01		3.3E+	01	
	10	S-01150	J. Jpn. Inst. Metals	1983	v. 047 p. 0382	G102-216018	4.5E+01		2.3E+	01	

- 42 glasses of 9 data sources are listed.
- By clicking the [Search Property DB] icon, the Glass Numbers of the corresponding glasses in the Property Database appear in the list.
- 3) Correlation between Q² and NBO ([XY Plot] window)



- An XY Plot of Q2/totalX (Si) vs. NBO/ [totalO] (O) is shown.
- With increasing Q², NBO fraction increases almost proportionally. If 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 rapidquenched glasses. This could be the reason why the plot-points are separated from the others.



🔯 INTERGLAD 8 : XY Plot × File Tools Help # 🖬 🝸 😝 😫 INTERGLAD 8: XY Plot /2 + a1× + a0 X = 63.17 Y = 3.131 80.0 a2: 7.926E-03 a1: 7.019E-01 a0: 9.482 70.0 : 8.813E-0 60.08 NBO / total O (0) 60.00 40.0 30.0 20.0 50.00 60.00 20.00 30.00 40.00 Li2O+Na2O+K2O mol% X axis Fitt Li2O+Na2 NBO / total O (O) Detai •K20 $y = a2X^2 + a1X + a0$ Delete Linear Undo * Delete a Source Zoom Reset Close

- 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 Q⁴.

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 Li₂O+Na₂O+K₂O vs. NBO/ [total O] (O). It is found that the NBO fraction increases proportionally with increasing the alkali content.