Examples of Use

Contents

Notes

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

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

2) Refer the User's Manual for detailed operation. Necessary chapters and sections are indicated under each example's title.

3) Number of searched data (Total Number) and data content in the [Data List of Property or Structure] window are different depending on the Version of INTERGLAD. So when the user tries the same example, the Total Number and the content may be different from those of the example described here. Ver.7.1.3.2.01−7.2.1.0.05 of INTERGLAD are used in these examples.

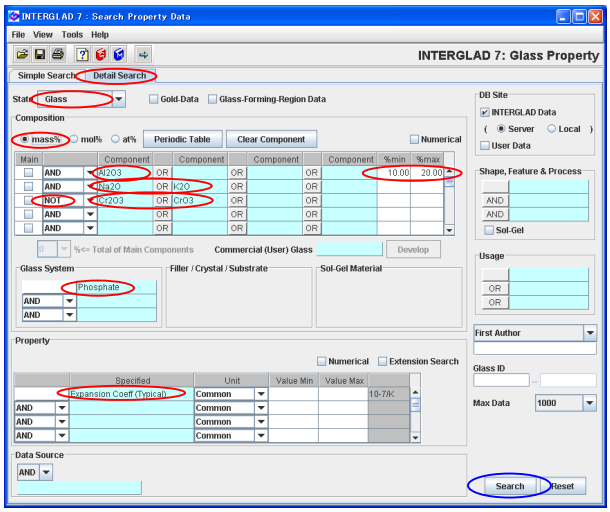
1. Search with a complicated composition
– Thermal expansion coefficient of phosphate glasses

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

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

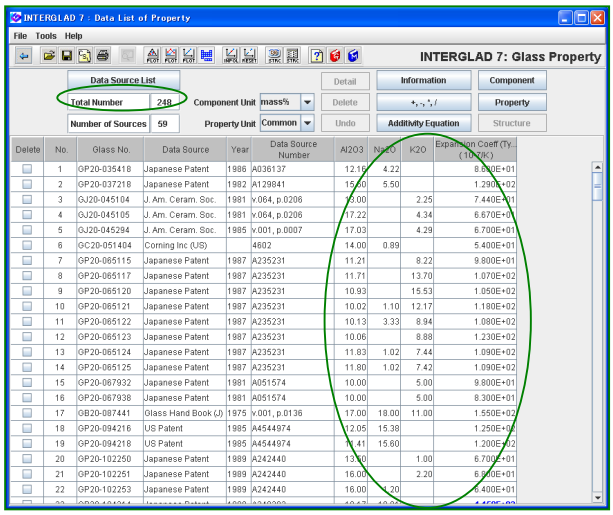
1) Specification of search conditions ([Search Property Data] window with [Detail Search] tag)

→ Search



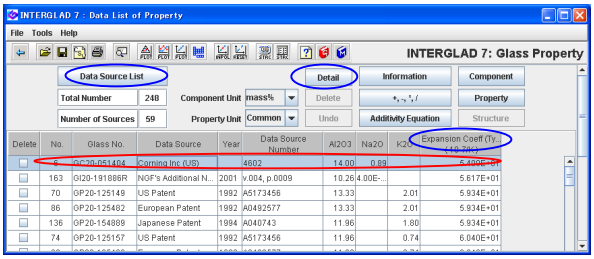
- Choose 'mass%' for the unit of composition. The default of the unit is mol%.
- Select 'Na2O' and 'K2O' in the same row with connection of 'OR.' In this case simultaneous selection is not available on the periodic table.
- Cr Oxides can be selected by selecting 'Cr' and 'O' on the Periodic Table.
-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

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

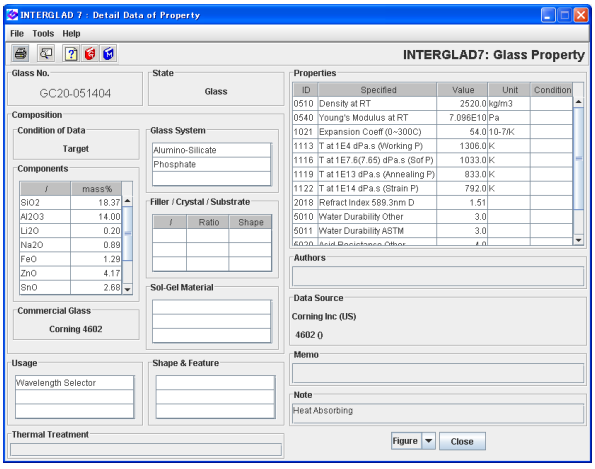


- Take notice of 'Total Number' of the Data Source.
- A table with values of components, property data etc., which are specified as the search conditions, appears.
- If necessary, analyze the dataset using Ternary Plot or XY Plot.

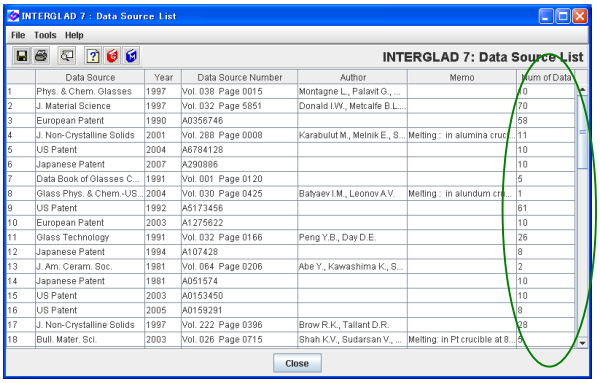
3) Utilization of the search result ([Detail Data of Property] window and [Data Source List] window)



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



[Detail Data of Property] window



[Data Source List] window

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

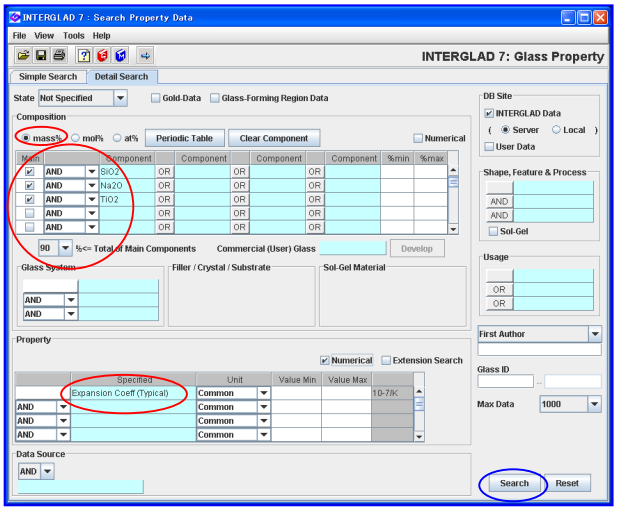
2. Ternary plot analysis of property data
– Thermal expansion coefficient of SiO_2-TiO_2-Na_2O glasses

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

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

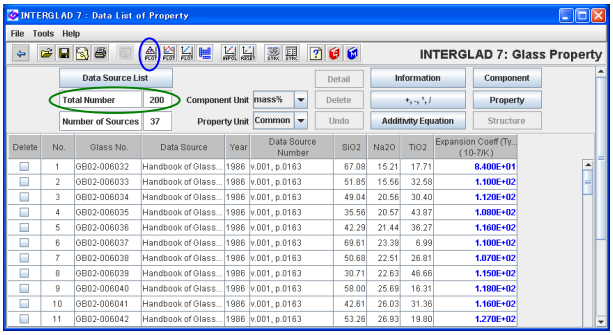
1) Specification of search conditions ([Search Property Data] window with [Detail Search] tag)

→ Search



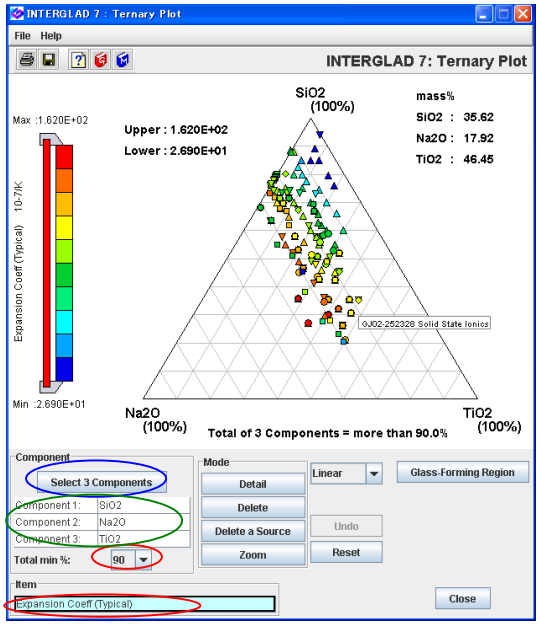
- Choose '90' mass% as the minimum Total of Main Components, SiO_2, TiO_2 and Na_2O.
- Select 'Expansion Coeff (Typical)' for the Specified of the Property.

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

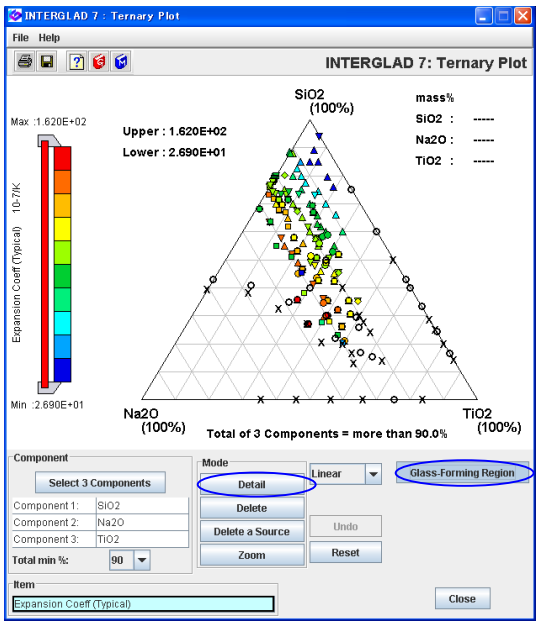


- 200 glasses are searched.

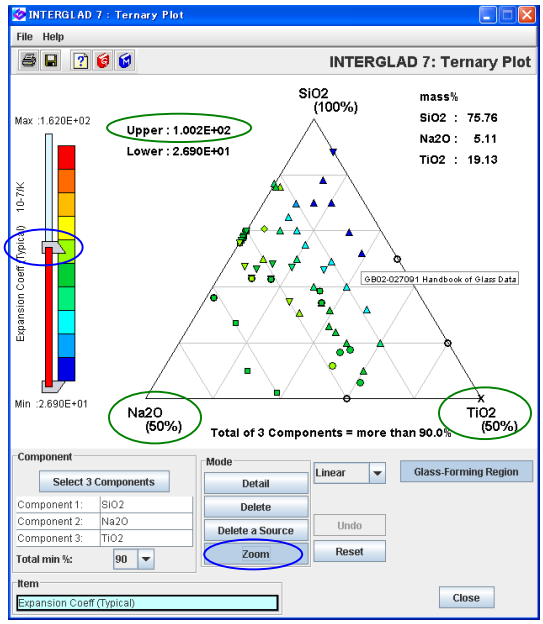
3) Ternary plot



- Open the [Ternary Plot] window by clicking the [Ternary Plot] icon. Select SiO_2, TiO_2 and Na_2O as 3 Components, '90' for the Total min%, and 'Expansion Coeff (Typical)' for the Item.
- Value levels of thermal expansion coefficients can be overviewed by plot-points with ten steps of colors in the diagram. Thermal expansion coefficient is high in the center region and decreases as the position moves to the upper right (near to SiO_2 100%).



- 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.



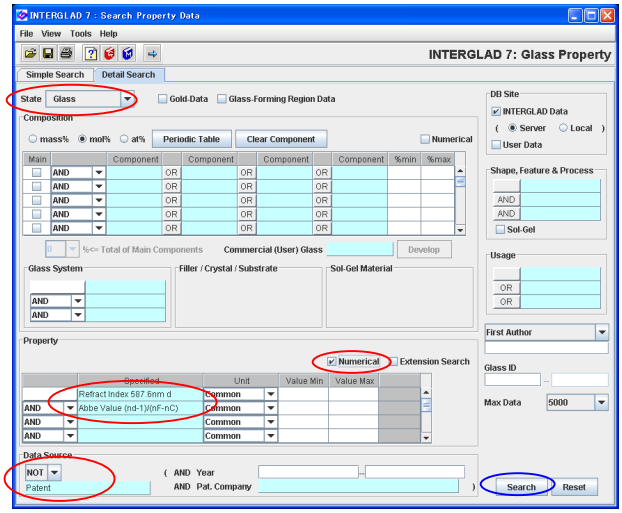
- By sliding the slider, property value range of glasses in the diagram can be changed. In the example of the left figure thermal expansion coefficient is limited to ≤ 100×10^{-7}/K, and the ternary diagram with SiO_2 (100%), Na_2O (50%), TiO_2 (50%) is shown by using the [Zoom] button.

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

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

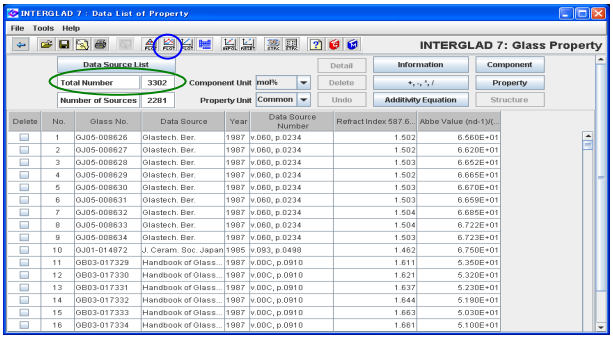
<Refer to B and C.2 of Chapter 3, and 2 and 3.2 of Chapter 4>

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



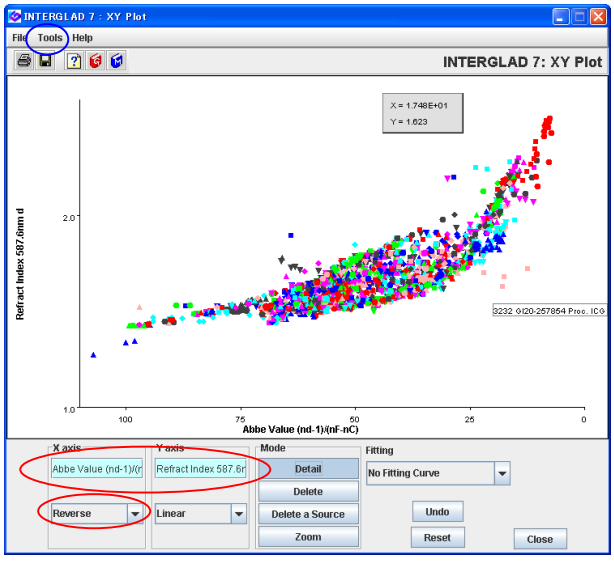
- Select 'Glass' for the State.
- As for refractive index, data measured by illuminants with various wavelengths are in the database. In this example, data by He d-line with 587.6nm are searched.
- Select '(nd-1)/(nF-nC)' for the Abbe value.
- Check in the [Numerical] checkbox.
- Select 'NOT Patent'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

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



- 3302 glasses are listed.

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



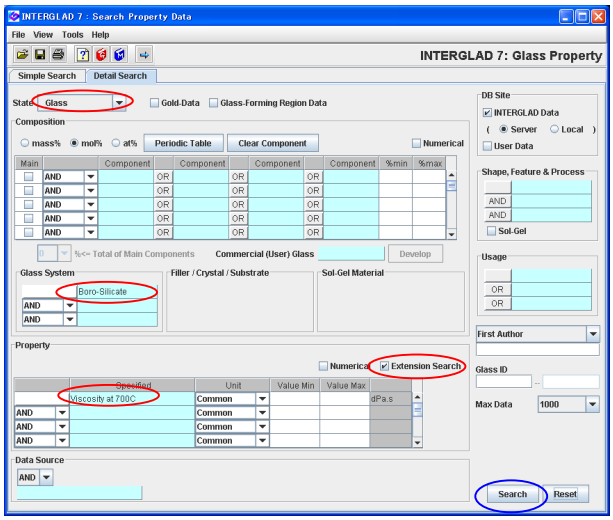
- From the [XY Plot] icon, an XY plot (Abbe value vs. refractive index) is shown. The distribution of Abbe values and refractive indexes of 3302 glasses is visualized.
- In this example, the style of x-axis for Abbe value is set to 'Reverse', and the ranges and scales are changed from the [Tools/ Option]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

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.

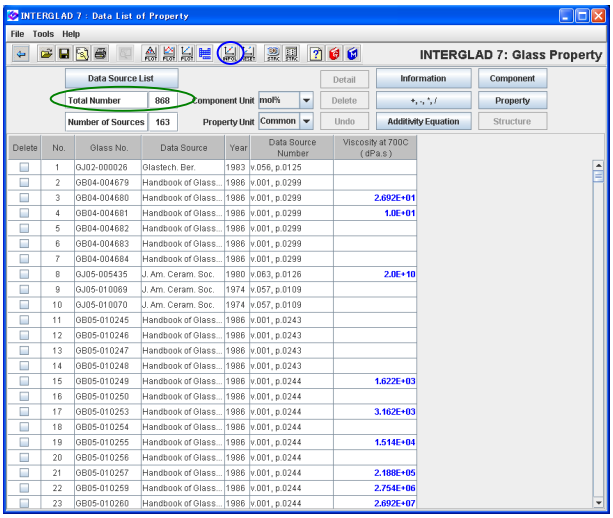
<Refer to B and C.3 of Chapter 3, and 2 and 3.3 of Chapter 4>

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



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

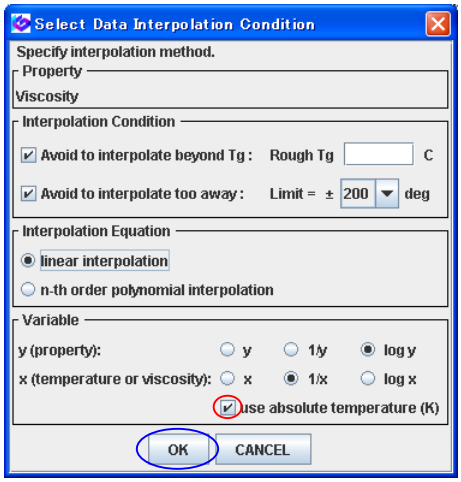
2) Search result ([Data List of Property] window)



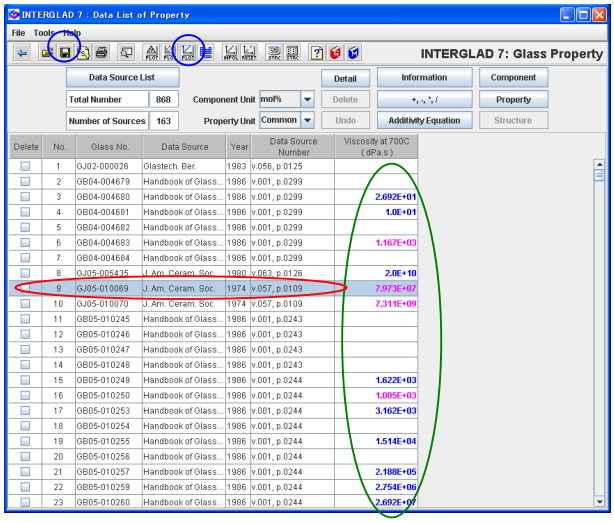
- As the search result, all the boro-silicate glasses which have registered viscosity data at high temperatures are listed. 868 glasses appear.
- When the search is performed using a keyword 'Viscosity (100-1000C),' all the glasses which have one or more data of viscosity at 100-1000°C are listed. In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

3) Data interpolation or extrapolation

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

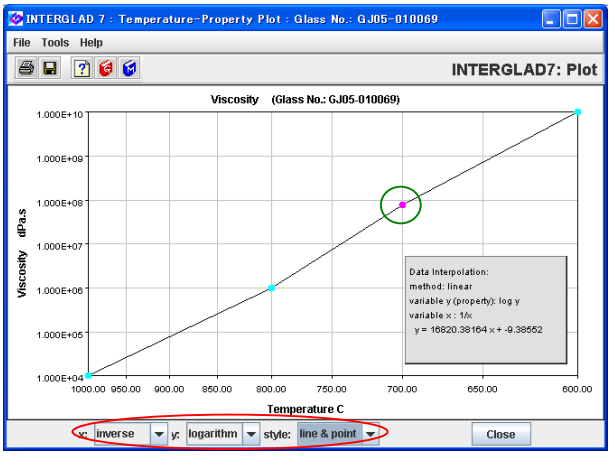


temperature (K)] checkbox. Then click the [OK] button.



- 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 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)

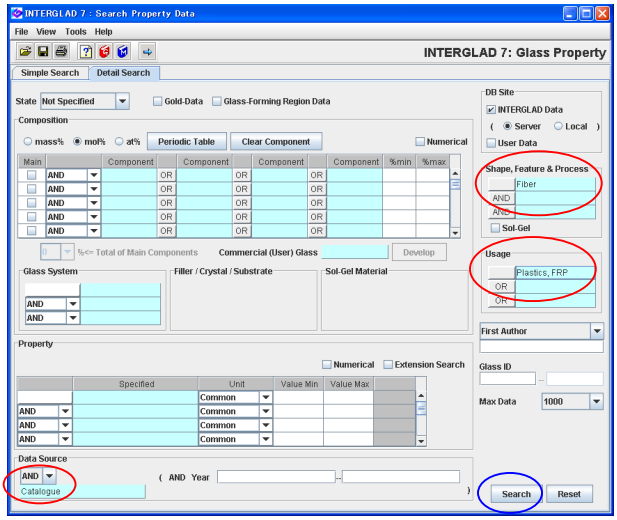
5. Search of commercial glasses – High strength glass fiber for FRP

Investigate commercial glasses of high strength glass fiber for FRP.

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

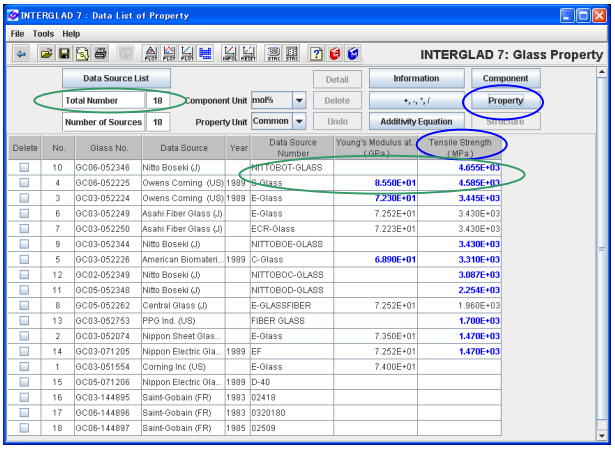
1) Specification of search conditions ([Search Property Data] window with [Detail Search] tag)

→ Search

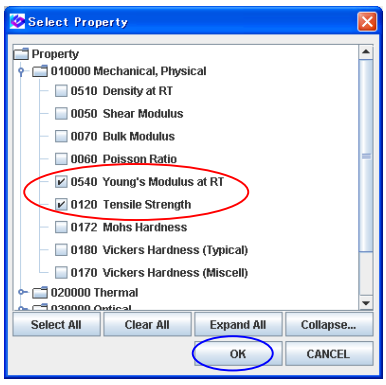


- Select 'Fiber' after opening 'Appearance/Shape/Linear' in the [Shape, Feature & Process] column.
- Select 'Plastics, FRP' in 'Material' by clicking the [Usage] column.
- Select 'Catalogue' for the [Data Source] column.

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



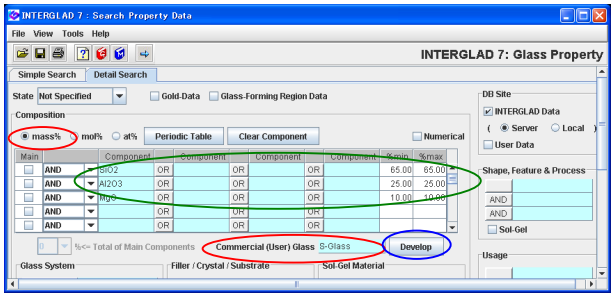
- 18 glasses are listed. These are found to be data of 10 manufacturers in the 'Data Source' column.
- Open the [Select Property] dialog box by clicking the [Property] button.
- Check in the 'Tensile Strength' and 'Young's Modulus at RT' checkboxes, and both the data are shown. Tensile strength and Young's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



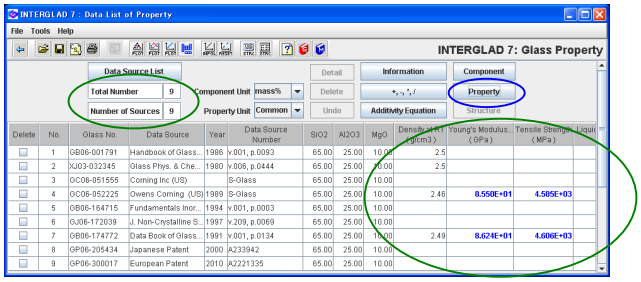
- By sorting the 'Tensile Strength' column, glasses with high strength can be found. (NITTOBO T-Glass and S-Glass are the highest.)

[Select Property] dialog box

3) Investigation of a searched glass

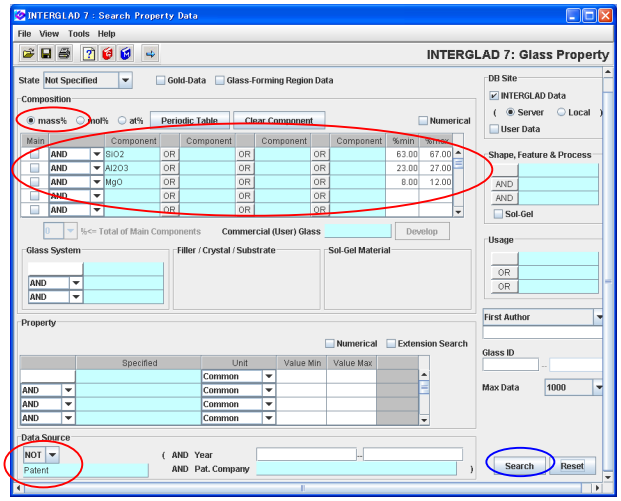


- Here S-glass with high tensile strength and high Young's modulus is investigated.
- Go back to the [Search Property Data] window, select 'S-Glass' in the [Commercial (User) Glass] column, and click the [Develop] button. Then search with no specification of the Data Source.
- In this case values of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

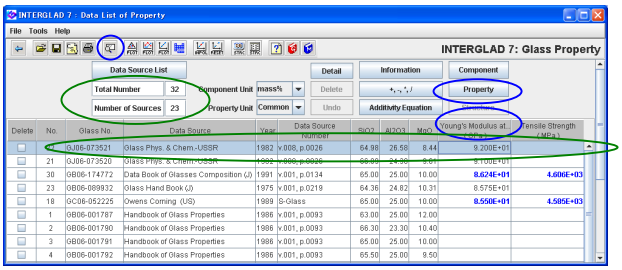


- 9 glasses (9 data sources) are listed. When the search is performed without clicking the [Develop] button, only 3 glasses are listed. By developing the composition, it is found that data of Journals, etc. besides catalogues are also searched.
- By clicking 'Select All' button in the [Select Property]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

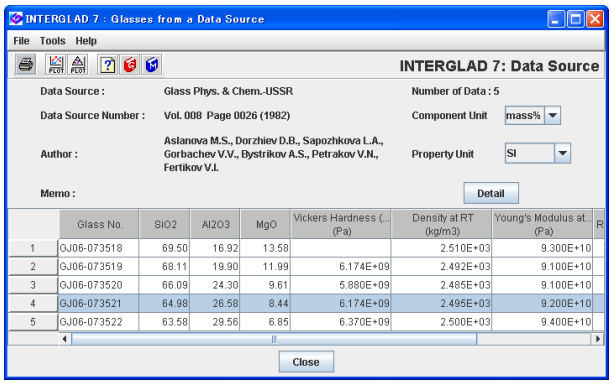
4) Investigation of data around S-Glass



- Information of glasses around S-Glass is collected.
- ±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.



[Glasses from a Data Source] window

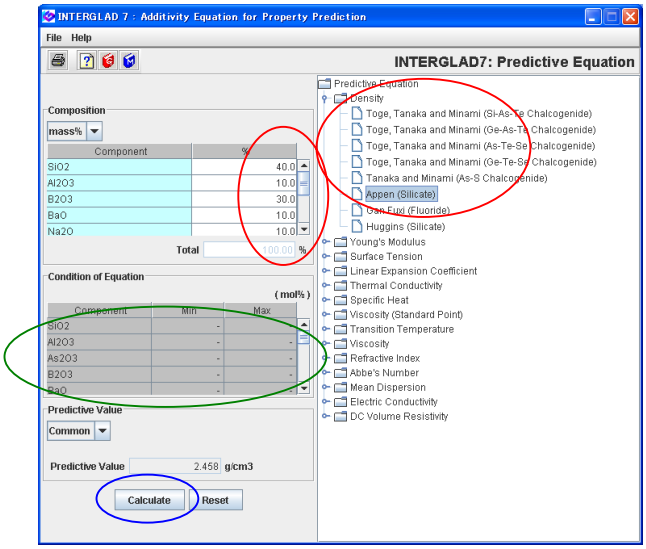
- Clicking the [Glasses from a Data Source] icon after selecting the glass GJ06-073521 with the highest Young's modulus opens the [Glasses from a Data Source] window of the glass. All the data in this data source can be checked.

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>

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

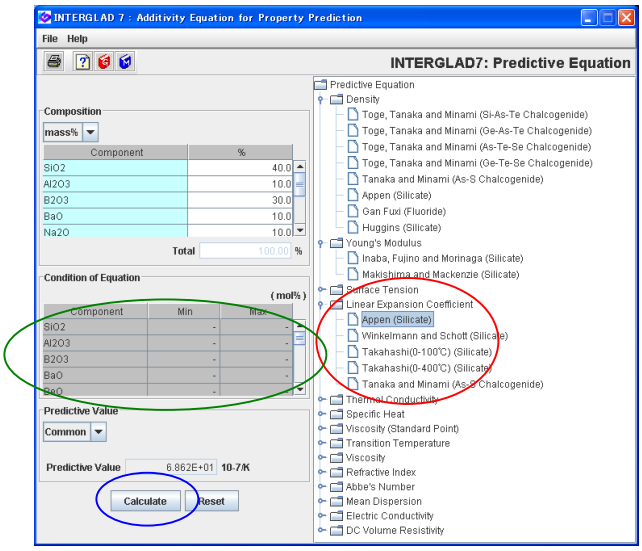


- Open the [Additivity Equation for Property Prediction] window, and select 'Appen(Silicate)' after developing 'Density' in the [Predictive Equation] menu on the right-hand part of the window .
- The [Condition of Equation] appears on the left-hand part. Check if the values of the components of glasses to be predicted are included in the condition.
- Select components required for the property prediction, and enter each value in the [Composition %] column. Plural components can be selected in one time by using the Ctrl key. In this example the component unit is mass%.
- After clicking the [Calculate] button, the predictive value 2.458 g/cm^3 appears in the [Predictive Value] column.

2) Prediction of thermal expansion coefficient

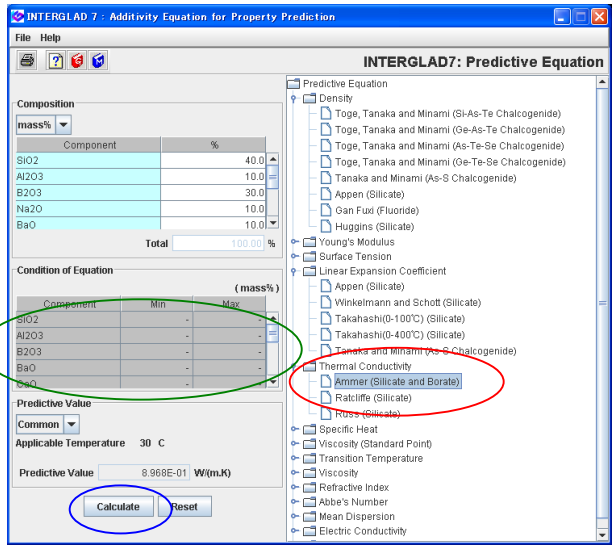
- In case of prediction of the other properties for the same composition, property prediction can be performed only by reselecting the property equation.
- Select 'Appen(Silicate)' after developing 'Linear Expansion Coefficient' in the [Predictive Equation]

menu.



- Clicking the [Calculate] button shows the predictive value 6.862×10^{-6} /K in the [Predictive Value] column.

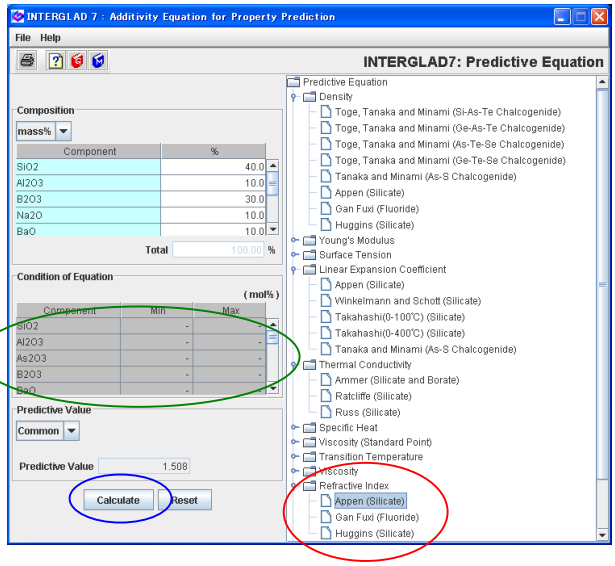
3) Prediction of thermal conductivity



- Select 'Ammer(Silicate and Borate)' after developing 'Thermal Conductivity' in the [Predictive Equation] menu.
- By clicking the [Calculate] button, the predictive value 8.968×10^{-1} W/(mK) (30°C) appears in the [Predictive Value] column.

- In this example, equations of 'Ratcliffe(Silicate)' and 'Russ(Silicate)' can also be used, and 8.349×10^{-1} W/(mK) (0°C) and 9.256×10^{-1} W/(mK) (0°C) are obtained respectively. The user can compare the results by the difference of additivity equations.

4) Prediction of refractive index



- Select 'Appen(Silicate)' after developing 'Refractive Index' in the [Predictive Equation] menu.
- By clicking the [Calculate] button, the predictive value 1.508 appears in the [Predictive Value] column.

- Predictive values of various properties can be calculated for a composition as described above, but in many cases calculations are not possible owing to various composition limitation of equations.

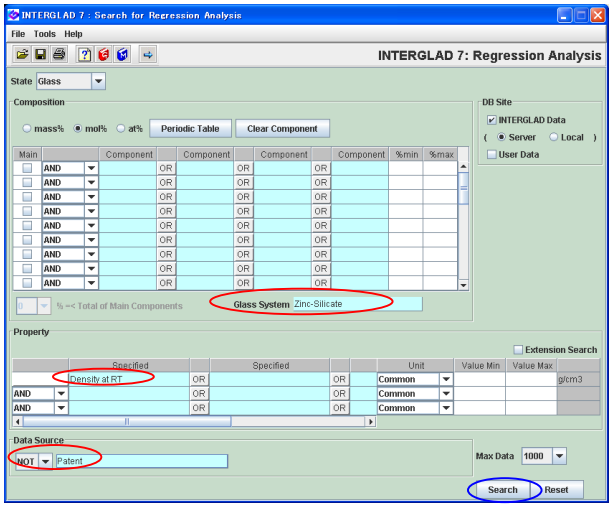
＜Refer to 1 of Chapter 6＞

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.

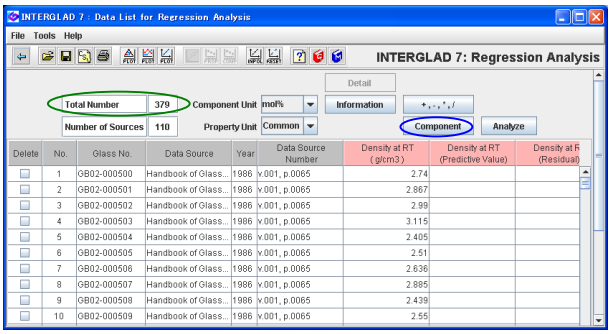
<Refer to D.2 of Chapter 3, 4.2-4.5 of Chapter 4>

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



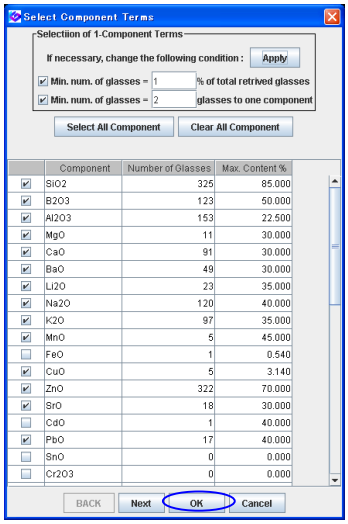
- Open the [Search for Regression Analysis] window.
- Select 'Glass' (default) for the State.
- Select 'Zinc-Silicate' for the Glass System, 'Density at RT' for the Property, and 'NOT Patent' for the Data Source.

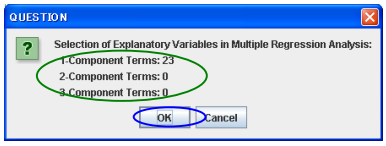
2) Search result ([Data List for Regression Analysis] window) → Selection of explanatory variables ([Selection of 1, 2, 3-Component Terms] dialog boxes)

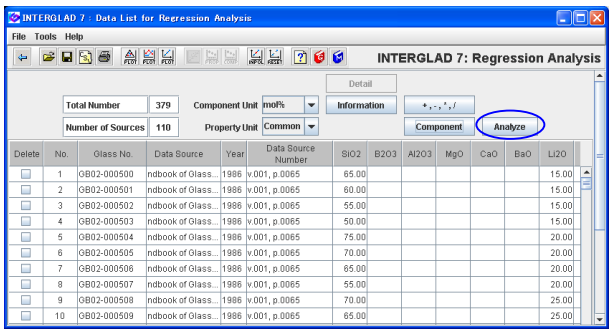


- 379 glasses are listed.
- Open the [Selection of 1, 2, 3-Component Terms] dialog boxes by clicking the [Component] button, and specify component terms for a multiple regression equation.
- In this example, click the [OK] button in the [Select Component Terms] dialog box for the Selection of 1-component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

  1-Component Terms: 23.

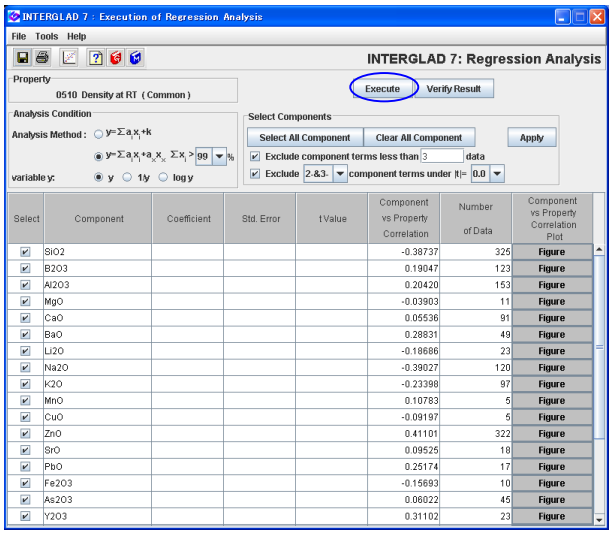






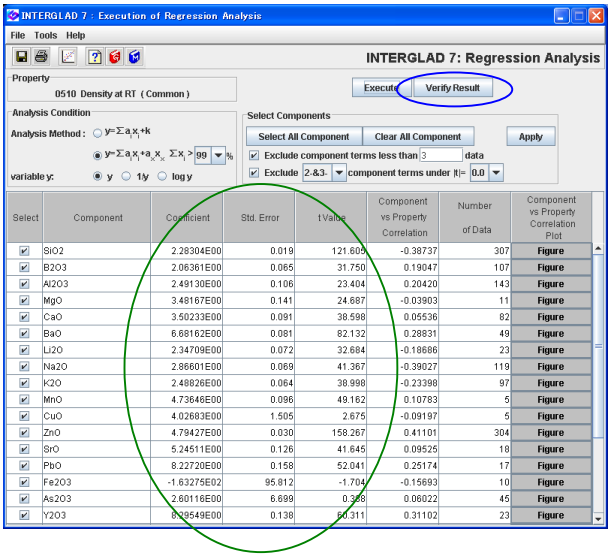
- By clicking the [Analyze] button, the [Execution of Regression Analysis] window opens.

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



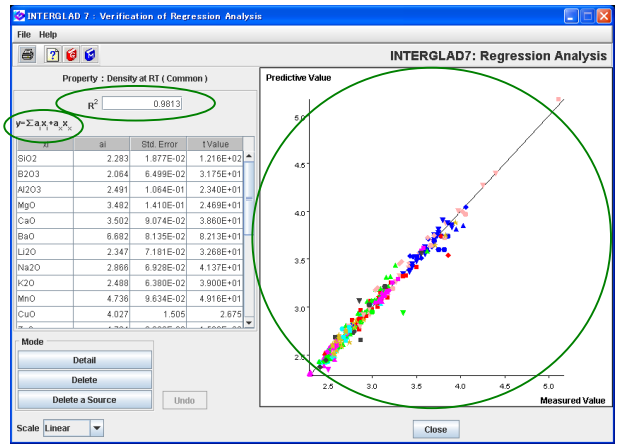
- Execute the multiple regression analysis at default setting by clicking the [Execute] button.

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



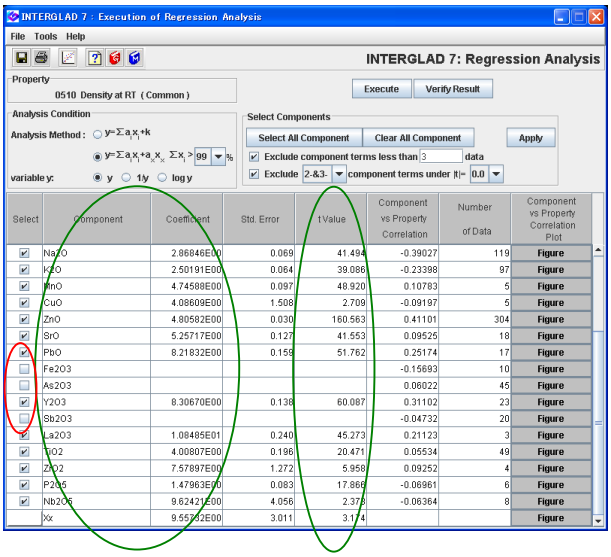
- The regression coefficients, the standard errors and t values appear in the table after the calculation.
- By clicking the [Verify Result] button, open the [Verification of Regression Analysis] window.

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

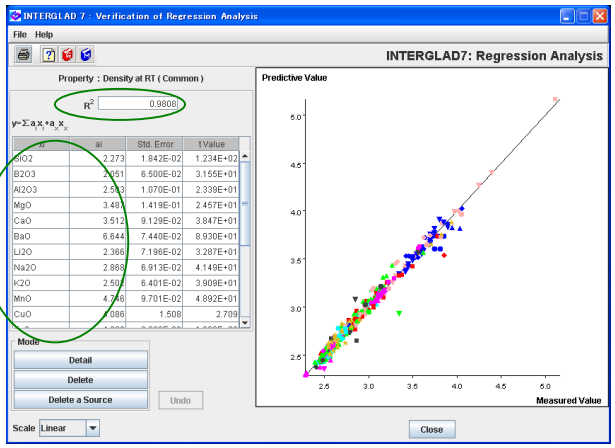


- In this example a high contribution rate R^2 (0.98) is obtained. The scattering of the plot-points is relatively small from the linear line y=x on the XY plot of the measured values vs. the predictive values. Value of ≥0.8 as the R^2 is recommended.

5) t value check → Recalculation



- Return to the [Execution of Regression Analysis] window, and check if the absolute value of t for each component term is low (<2) or not. $|t|$ value is recommended to be ≥2.
- In this example, $|t|$ of Fe_2O_3, As_2O_3 and Sb_2O_3 are <2. First, delete ✓ in the checkboxes of As_2O and Sb_2O_3 with $|t|$<1, and recalculate. Second, delete ✓ in the checkbox of Fe_2O_3 with $|t|$<2, and recalculate. By these procedures the component terms with $|t|$<2 are removed from the multiple regression equation.



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

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

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

Analysis] window and the [Verification of Regression Analysis] window

- The obtained equation:

  Density at RT (g/cm^3) = 2.273× (SiO_2) + 2.051×(B_2O_3) + 2.503×(Al_2O_3) + ·····

  (SiO_2), (B_2O_3) ,····· : 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.

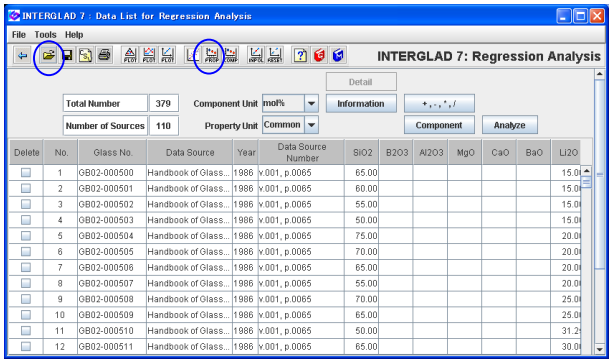
8. Property prediction by multiple regression analysis — Density of zinc-silicate glasses

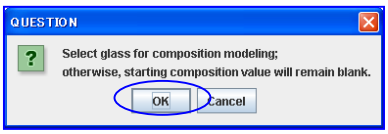
Predict density at RT of a glass with SiO_2 60%, Li_2O 20% and ZnO 20% (mol%).

<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 → Transit to the [Property Prediction] window

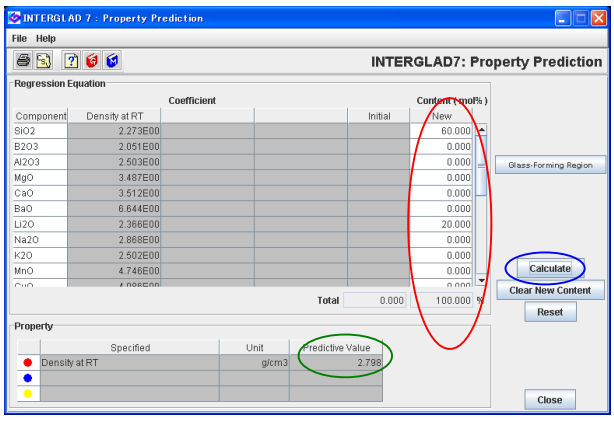




- Open a [Data List for Regression Analysis] window, and by clicking the [Open] icon open the [Data List for Regression Analysis] window of the result of 7. saved in the folder of the user's PC.

- 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.

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^3.

9. Composition optimization by multiple regression analysis

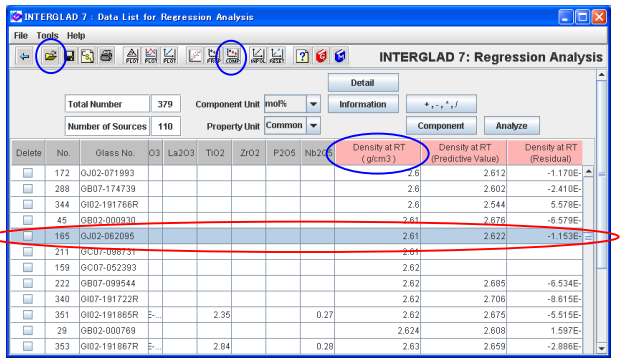
— Zinc-silicate glass with a specified density

Obtain a composition of zinc-silicate glass with 2.6 g/cm³ of density at RT. The components of the glass are SiO_2, B_2O_3, Na_2O, and ZnO.

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

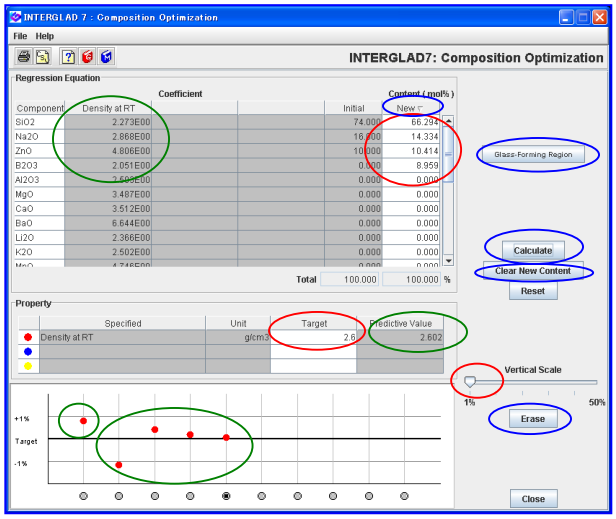
The multiple regression equation obtained in 7. is used because of the same zinc-silicate glass system.

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



- Open a [Data List for Regression Analysis] window, and by clicking the [Open] icon open the [Data List for Regression Analysis] window of the result of 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/cm³ of density as a model.
- By clicking the [COMP] icon, the [Composition Optimization] window opens.

2) Composition optimization

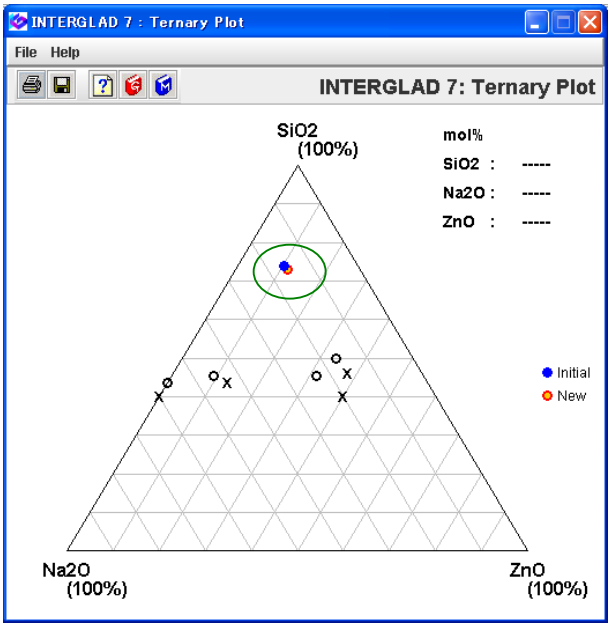


- Enter the target value 2.6 in the [Target] cell of the [Property] column, and click the [Calculate] button. The calculated value appears in the [Predictive Value] cell. In the graph on the bottom part of the window, the difference between the value of the model glass and the target is shown as a point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

- By clicking the [Clear New Content] button, the values in the [New] cells become null. Enter component values in the [New] cells of SiO_2, B_2O_3, Na_2O and ZnO referring the initial (model) values. In this example enter the close integral numbers of the initial values for SiO_2, B_2O_3 and ZnO, and 10 for B_2O_3. 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^3 in case of the following composition.
  The composition: SiO_2 66.3%, B_2O_3 9.0%, Na_2O 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



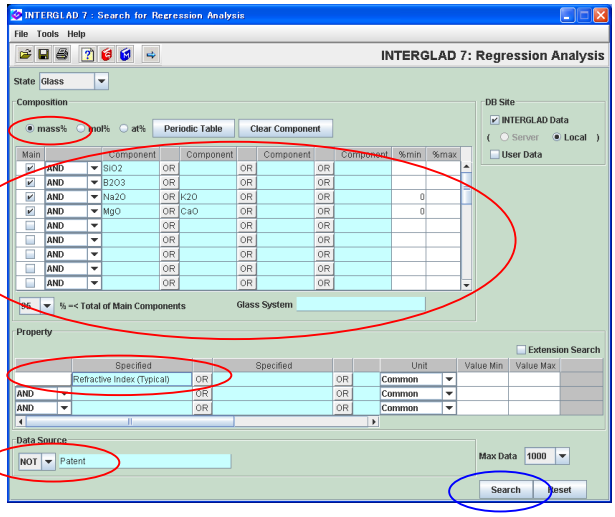
- By using the [Glass-Forming Region] button, the [New] and [Initial] composition can be shown in the [Ternary Plot] window. In this example the [Initial] and [New] compositions are plotted with the glass-forming region data of SiO_2-Na_2O-ZnO system.
- Glass-forming region data of the Ternary Plot are 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_2-B_2O_3-R_2O-RO system with the following composition. SiO_2 65%, B_2O_3 10%, MgO 5%, CaO 4%, Na_2O 7%, $K2O$ 5%, Al_2O_3 4% (mass%).

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

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



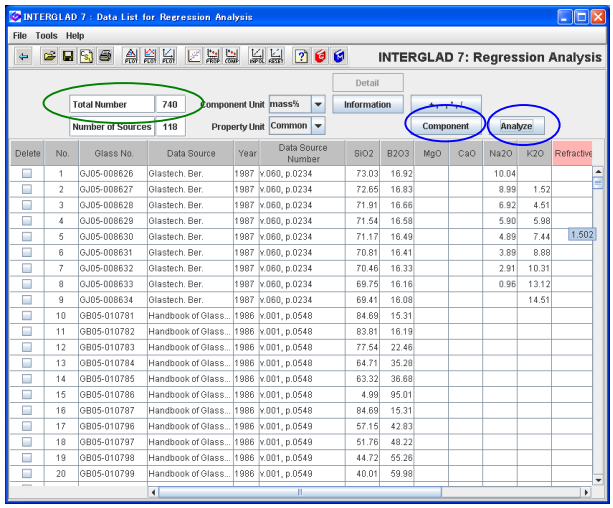
- Specify the following condition of composition.

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

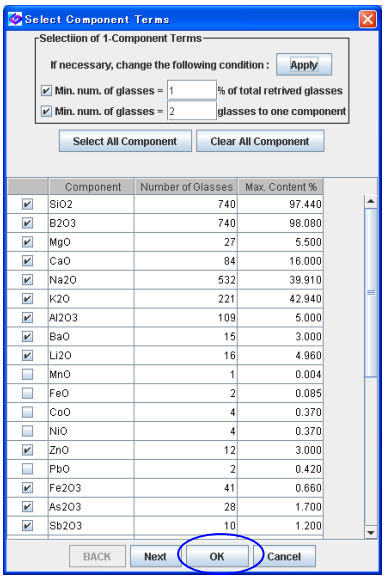
  $+ (MgO \text{ or } CaO \geq 0) \geq 95$ mass%.
- Select 'Refraction Index (Typical)' for the Property, and 'NOT Patent' for the Data Source.

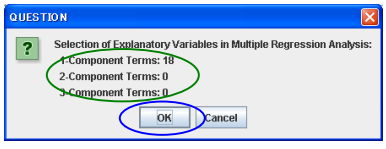
2) Search result ([Data List for Regression Analysis] window)

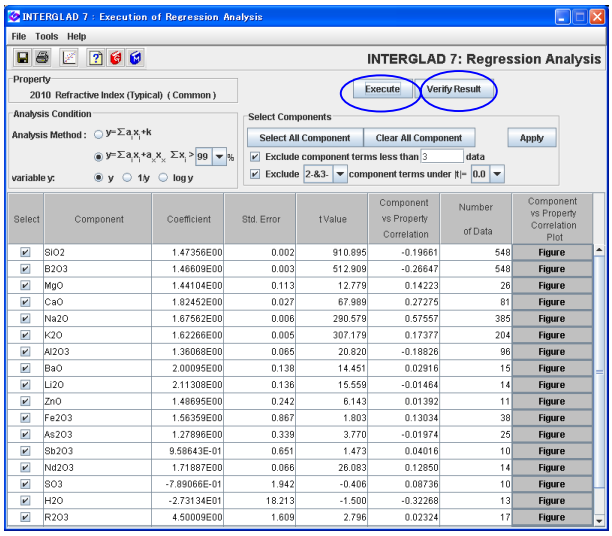
3)



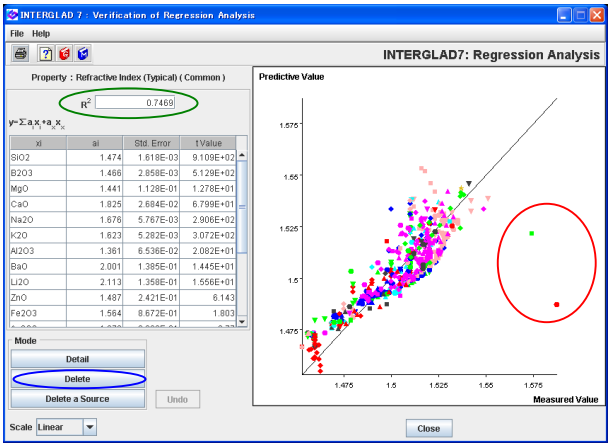
- 740 glasses are listed.
- First, regression analysis by a linear equation is carried out for comparison.
- In case of selection of only 1-component terms at default setting, 18 component terms are selected.



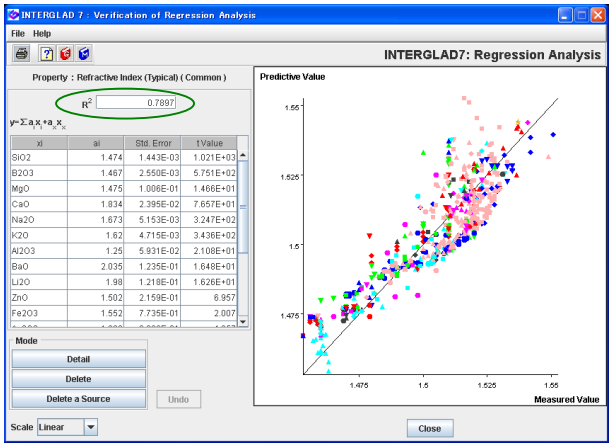




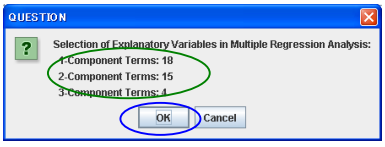
- Execute the regression analysis in the [Execution of Regression Analysis] window, and open the [Verification of Regression Analysis] window. The contribution rate R^2 is relatively low, 0.7469, and the plot-points have some difference from y=x.



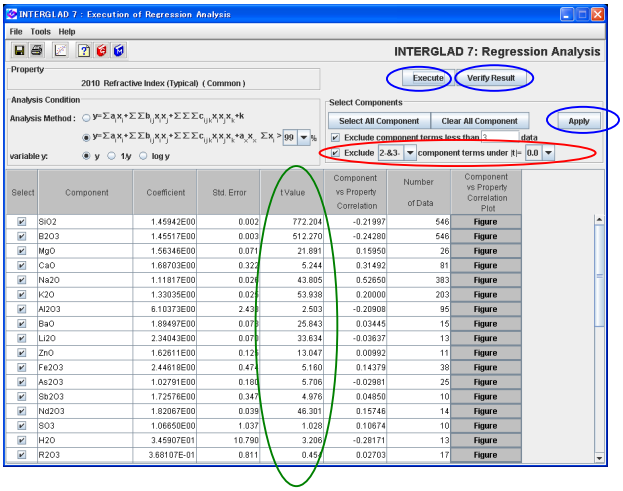
- After removing 2 separated plot-points from y=x, execute the regression analysis again. The obtained R^2 is still low, 0.7897. So this linear regression equation is not sufficient for good prediction.



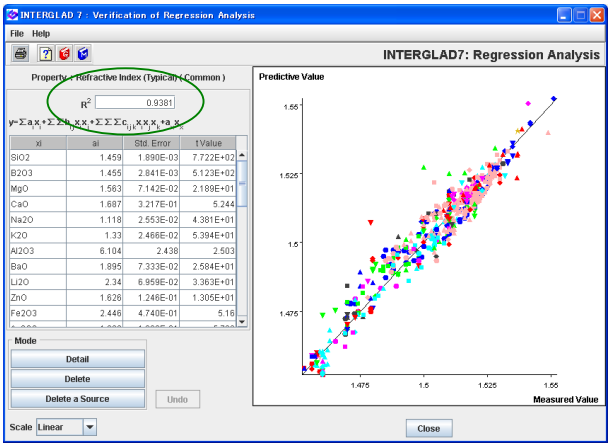
4) Regression analysis by a cubic equation



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

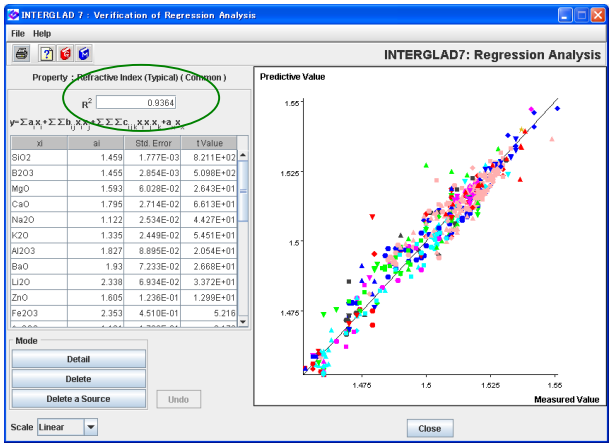


- Execute the regression analysis in the [Execution of Regression Analysis] window, and open the [Verification of Regression Analysis] window. R^2 is found to be 0.9381, a good result.
- Check t values in the [Execution of Regression Analysis] window. Component terms with $|t|<2$ are 11 (1-component terms: 2, 2-component terms: 8, 3-component terms: 1).

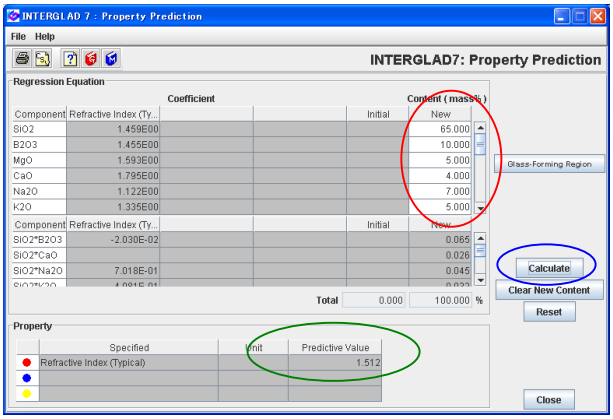


- In the third row of the [Select Components] column, set up an excluding condition of component terms with low $|t|$ values, click the [Apply] button, and click the [Execute] button. Exclude not in one time, step by step as follows.
  1) Exclude '2&3' component terms under $|t|$ = '1.0.'
  2) Exclude '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 ≥2.0, and R^2=0.9364.



5) Property prediction ([Property Prediction] window)



- Return to the [Data List for Regression Analysis] window, and open the [Property Prediction] window from the [PROP] icon.
- Enter component values (SiO_2 65%, B_2O_3 10%, MgO 5%, CaO 4%, Na_2O 7%, K_2O 5% Al_2O_3 4%) in the [New] cells of the [Regression Equation/ Content]

column, and click the [Calculate] button.

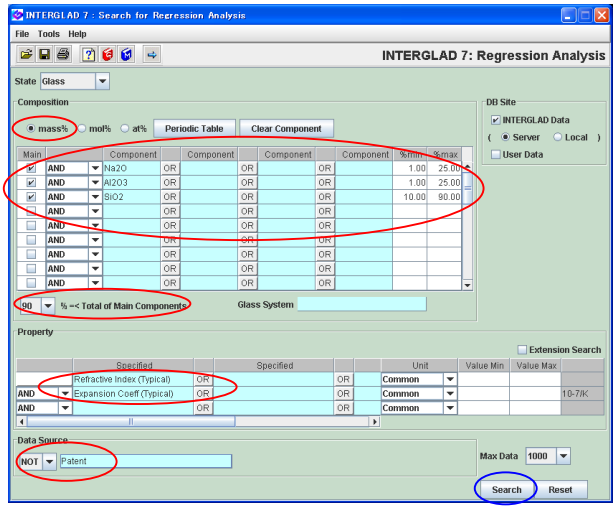
- 1.512 for the calculated refractive index value appears in the [Predictive Value] cell of the [Property] column.

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

Optimize composition of soda alumino-silicate glass with 80×10^{-7}/°C of thermal expansion coefficient and 1.49 of refractive index.

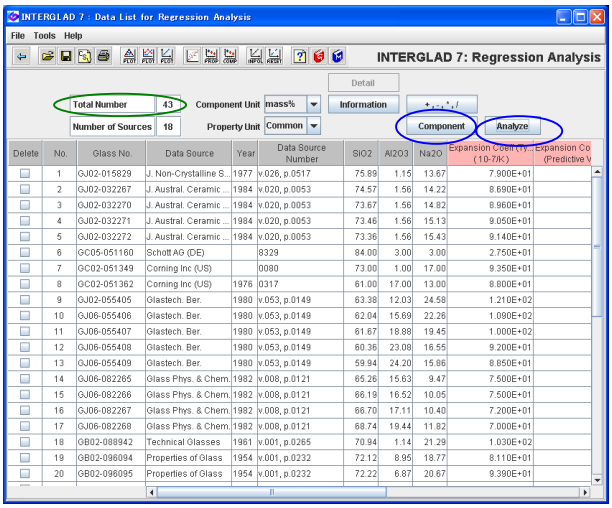
<Refer to D.3 of Chapter 3, 4.2-4.5 and 4.7 of Chapter 4>

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



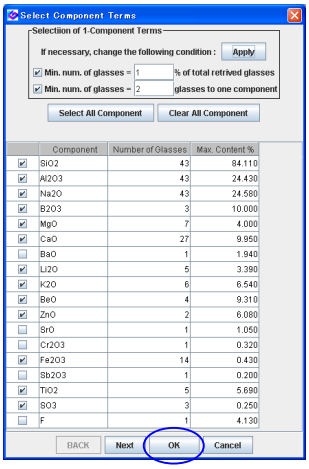
- Specify a wide composition condition to collect many related data. For example set up composition conditions as follows. $10 \leq SiO_2 \leq 90\%$, $1 \leq Al_2O_3 \leq 25\%$, $1 \leq Na_2O \leq 25\%$, $SiO_2+Al_2O_3+Na_2O \geq 90\%$ (mass%).
- Select 'Expansion Coeff (Typical)' and 'Refractive Index (Typical) for the Property. Specifying properties with 'Typical' is effective to collect many data.
- Select 'NOT Patent' for the Data Source in this example.

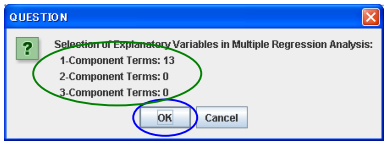
2) Search result ([Data List for Regression Analysis] window)



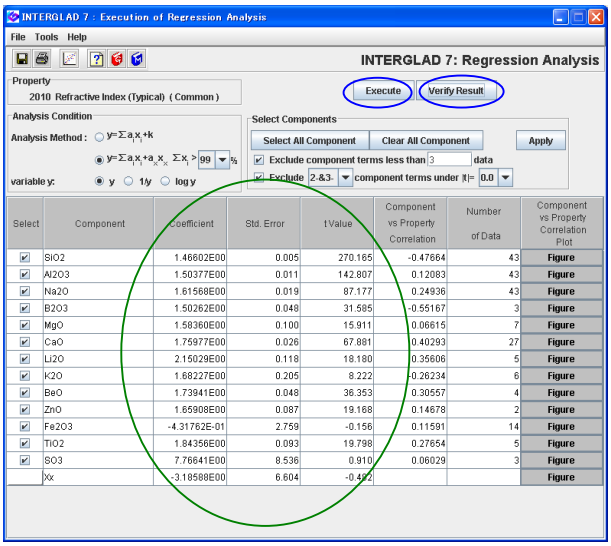
- 43 glasses are listed.

3) Regression analysis by a linear equation

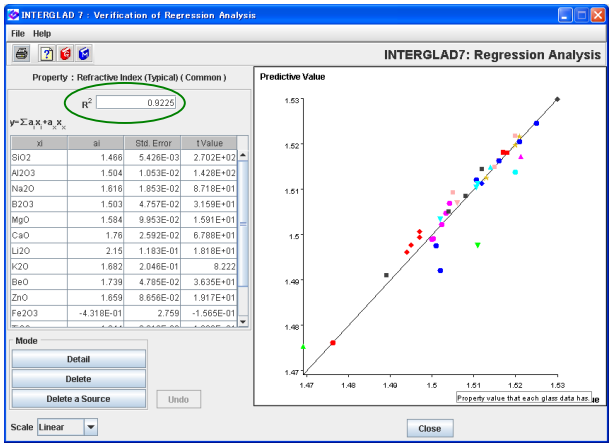




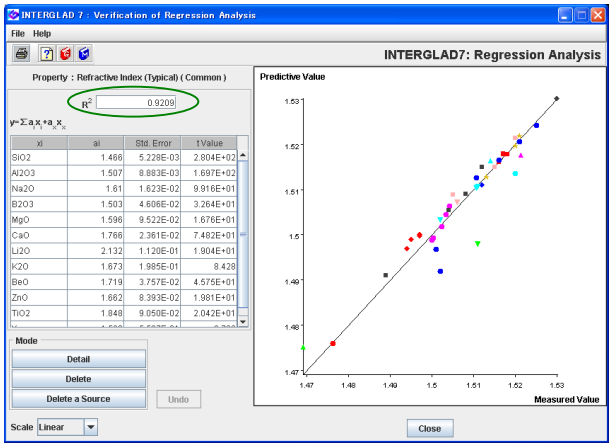
- Open the [Select Component Terms (1-Component Terms)] dialog box by clicking the [Component] button, and click the [OK] button at default setting.
- Check that the 1-component terms are 13, and click the [OK] button.



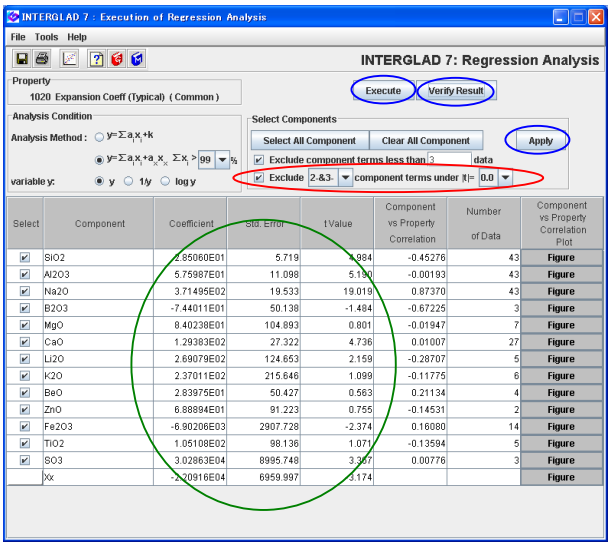
- After clicking the [Analyze] button in the [Data List for Regression Analysis] window, two [Execution of Regression Analysis] windows of refractive index and thermal expansion coefficient appear one upon another.
- First, click the [Execute] button in the window of refractive index. In each [Question]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



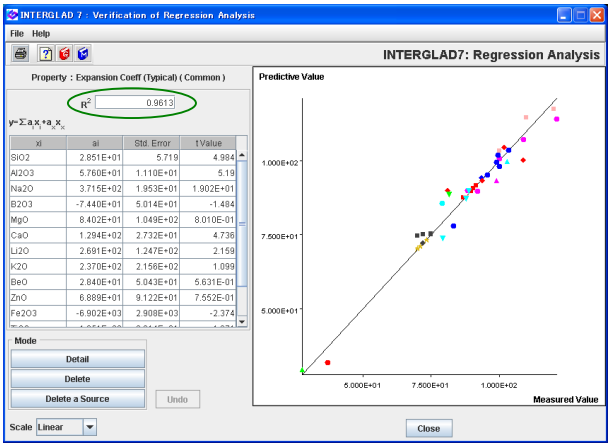
- Open the [Verification of Regression Analysis] window by clicking the [Verify Result] button.
- Note that the contribution factor R^2 is 0.9225, which is a good value over 0.9.
- Check t values. Component terms with $|t|<2$ are 2.



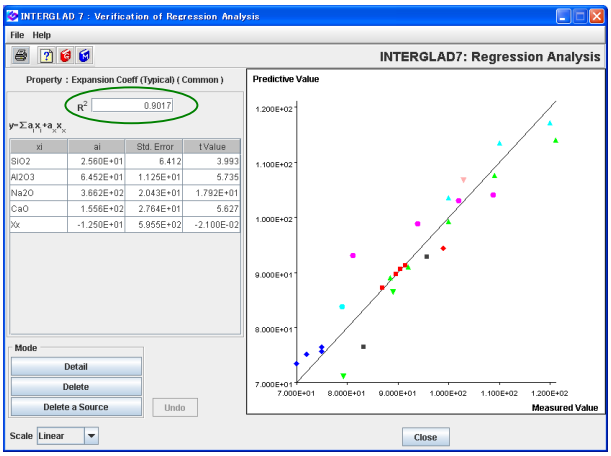
- Delete checks in the [Select] checkboxes of the component terms with low $|t|$ value, i.e. Fe_2O_3 with -0.156, SO_3 with 0.910, and execute again. Then all the $|t|$ values become ≥ 2, and R^2 is 0.9209. By this operation the regression equation of refractive index is completed.



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



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

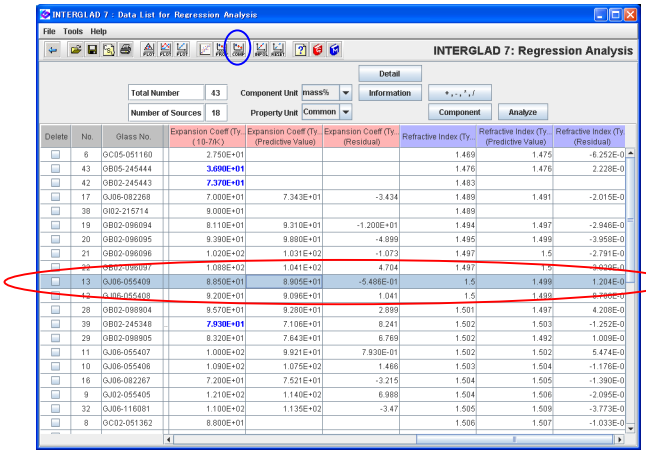


- In the third row of the [Select Component] column, set up an excluding condition of component terms with low $|t|$ values, click the [Apply] button, and click the [Execute] button in the following order.
  1) Exclude 'all' component terms under $|t|$ = '1.0.'
  2) Exclude 'all' component terms under $|t|$ = '1.0' again.

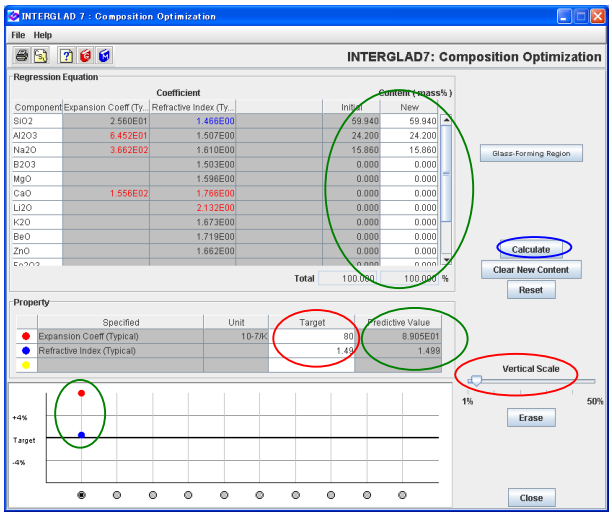
3) Exclude 'all' component terms under $|t| = 1.5$.'

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

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



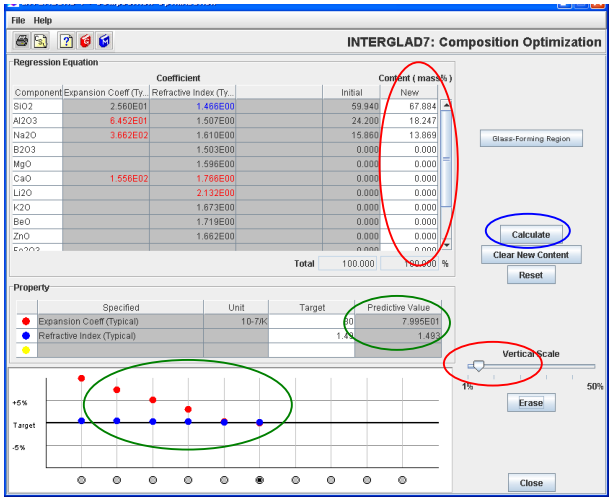
- Return to the [Data List for Regression Analysis] window, and select a glass with near properties to the target property. In this example select a glass row of No. 55409 in which the predictive value of Expansion Coeff is the nearest to the target value. Click the [COMP] icon, and open the [Composition 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^{-7}/°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_2 content and decreasing

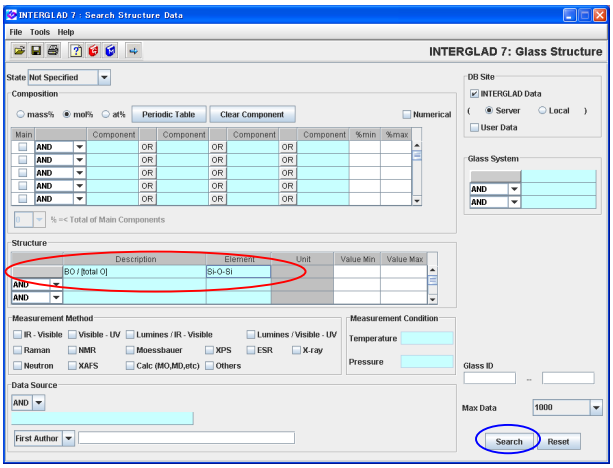
Al_2O_3 and Na_2O contents with high regression coefficients of thermal expansion.

- An optimized composition is as follows: SiO_2 67.88%, Al_2O_3 18.25%, Na_2O 13.87%. This glass has 79.95×10^{-7}/°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

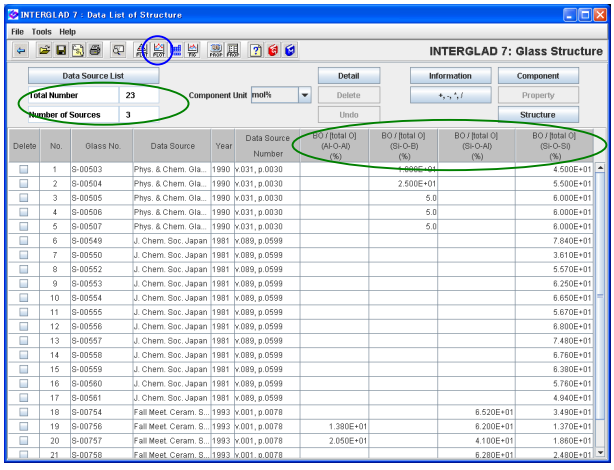
<Refer to E of Chapter 3, and 5 of Chapter 4>

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



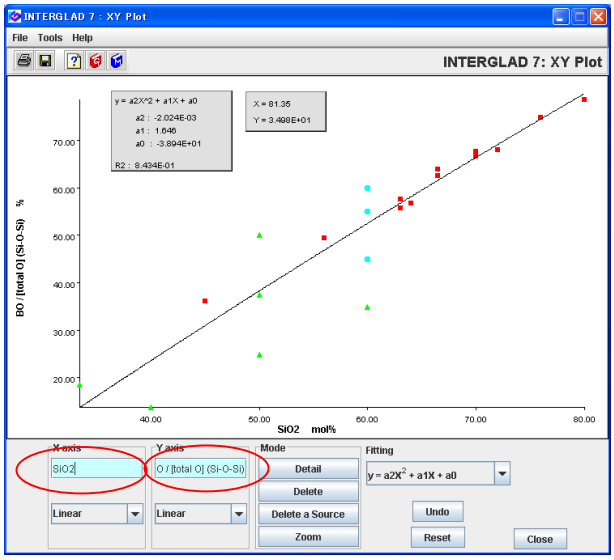
- Specify 'BO/ [totalO]' for the Description, and Si-O-Si for the Element in the [Structure] column. 'BO/ [totalO] (Si-O-Si)' means fraction of bridging oxygen with Si to the total oxygen.

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



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

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

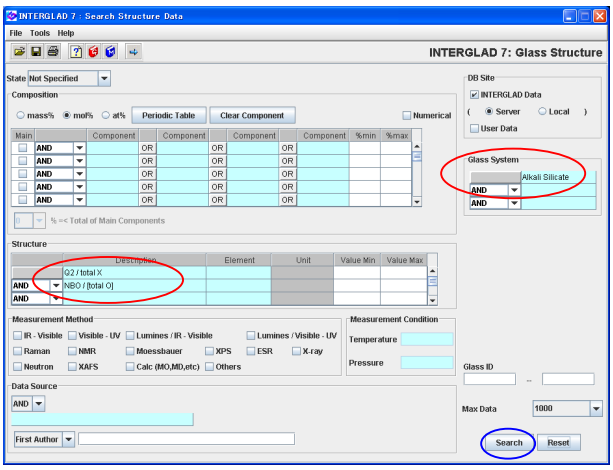


- An XY plot of SiO_2 content vs. BO/[total O] (Si-O-Si) is shown.
- As composition is not specified in this example, various components are contained. It is found that the bridging oxygen increases with increasing SiO_2 content.

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

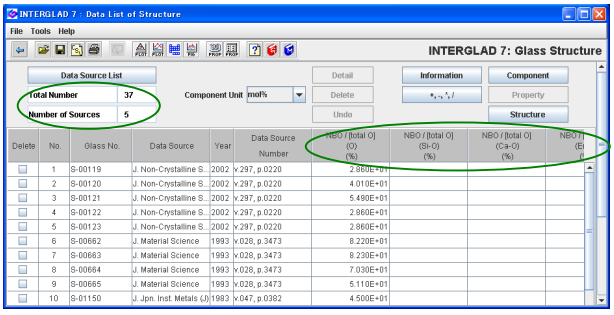
<Refer to E of Chapter 3, and 5 of Chapter 4>

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



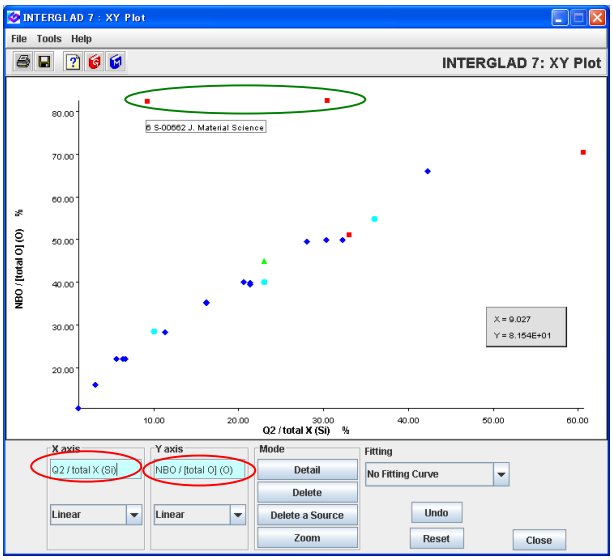
- Specify 'Alkali Silicate' for the Glass System.
  Select 'Q2/totalX' of the 'Qn Distribution' and 'NBO/ [totalO]' both in the 'Bridging Oxygen Information' for the Description of the [Structure] column. 'Q2/totalX' means Q^2 fraction in tetrahedra XO_4. 'NBO/ [totalO]' means fraction of non-bridging oxygen to the total oxygen.

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

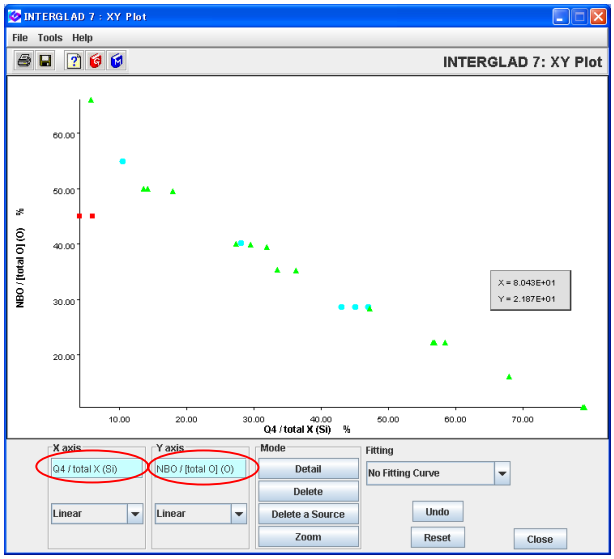


- 37 glasses of 5data sources are listed.
- As NBO/ [totalO], not only NBO/ [totalO] (O) but also those of (Si-O) and (Ca-O) are listed. As Q2/ totalX, Q2/ totalX (Al) is also listed besides that of (Si).

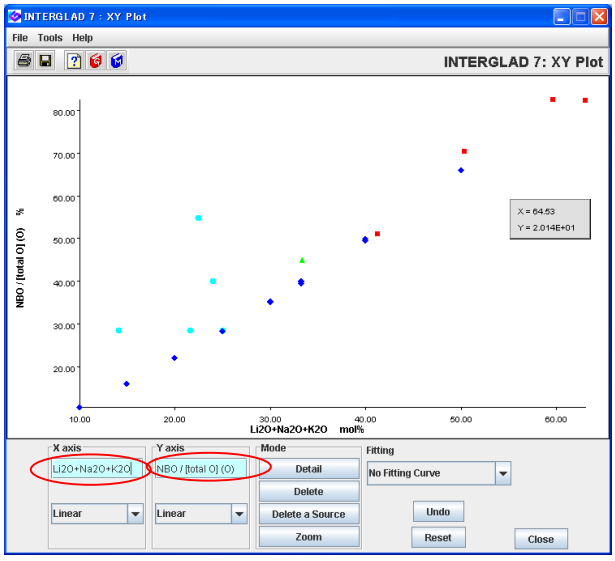
3) Correlation between Q^2 and NBO ([XY Plot] window)



- An XY Plot of Q2/totalX(Si) vs. NBO/ [totalO](O) is shown.
- With increasing Q^2, NBO fraction increases almost proportionally. When the 2 glasses at separated positions from the others are checked in the [Detail Data of Property] windows of the corresponding Glass No. (Property), it is found that they are both rapid-quenched glasses. This is the reason why the plot-points are separated from the others.



- For comparison, an XY Plot of Q4/totalX(Si) vs. NBO/ [totalO](O) is shown.
- The figure shows a reasonable tendency that NBO fraction decreases with increasing Q^4.



- All the searched glasses in this example contain alkali components. Relation between content of alkali oxides and fraction of non-bridging oxygen is checked in this XY Plot of content of $Li_2O+Na_2O+K_2O$ vs. NBO/ [totalO](O). It is found that the NBO fraction increases proportionally with increasing the alkali content.