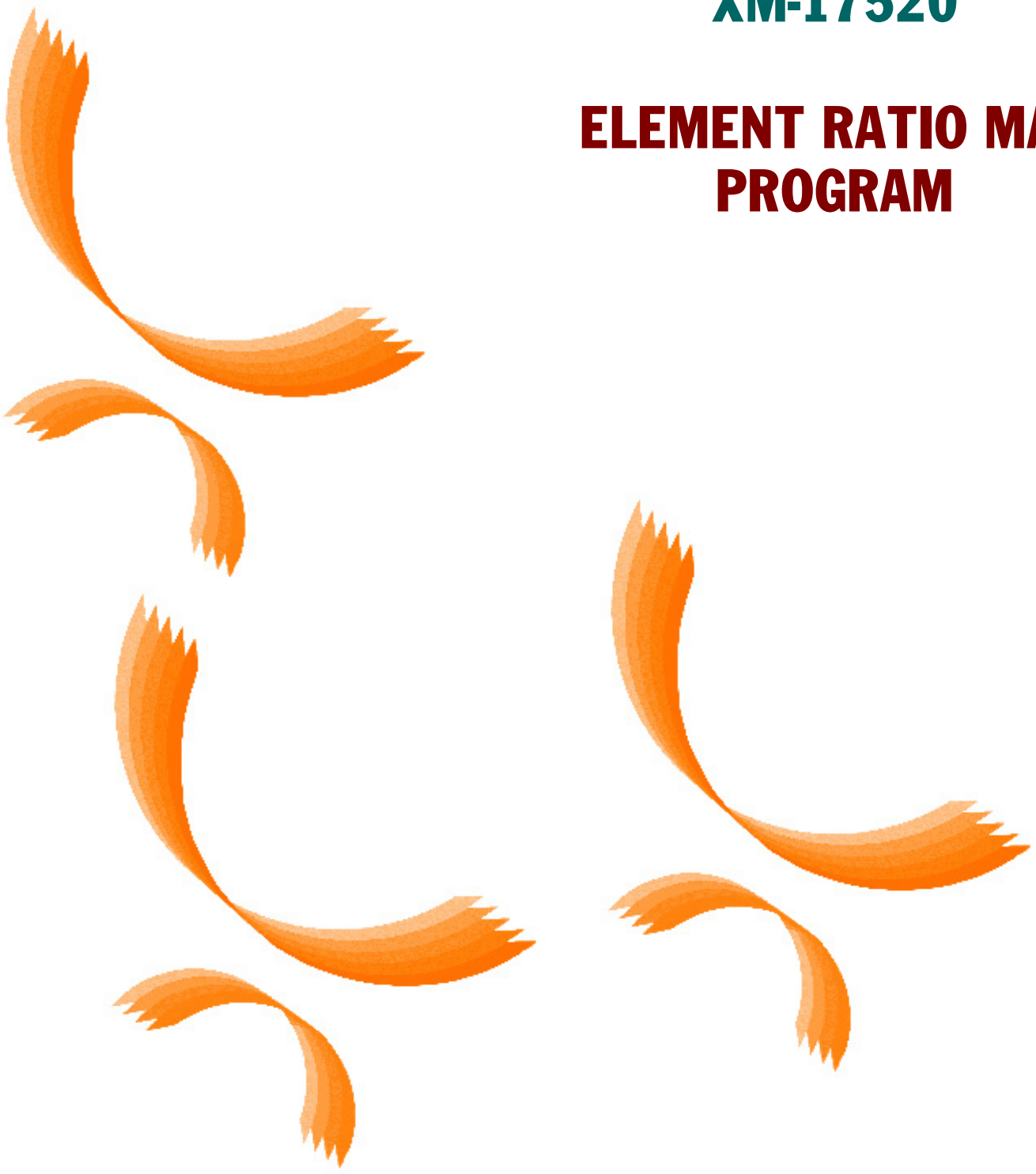
XM-17520

ELEMENT RATIO MAP PROGRAM



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XM-17520

ELEMENT RATIO MAP PROGRAM

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1 GENERAL

This element ratio map program is optional software for JXA-8100/8200's map analysis program.

It calculates the element ratio between each component at each point on a map, based on one or multiple displayed maps, and displays the result map and the calculation conditions on the screen. It permits any one of four modes, mass concentration as a metal (single element), atomic concentration as a metal, mass concentration as a compound, and molecular concentration as a compound, to be selected, enabling an element ratio map to be calculated and displayed. The detailed calculation conditions can also be printed out.
In addition, the result map can be stored as a file. By using these functions, map data can be utilized effectively in various fields, such as compilation of a map of atomic number ratio in a mineral specimen.

The following is an explanation of the way in which an element ratio map is calculated.

$$M = \frac{K_1 \times X_1 + K_2 \times X_2 \cdots + K_x \times X_x}{L_1 \times X_1 + L_2 \times X_2 \cdots + L_x \times X_x} \quad \text{..... (1)}$$

Equation (1) is the basic equation for performing element ratio calculations. This calculation is performed at each point on the map. Here, X_i is the mass concentration or atomic concentration as a metal, or the mass concentration or molecular concentration as a compound, for the ith element pertaining to $X_1 - X_x$.
K_i and L_i are factors pertaining to each component X_i.

- **In the case where only the intensity ratio is calculated, X_i in Equation (1) becomes as follows.**

$$X_i = I_i \quad \text{..... (2)}$$

where I_i = the intensity of component i (i = 1, ... x)

- **In the case where the element ratio as a metal is calculated, X_i in Equation (1) becomes as follows.**

  - When the mass concentration ratio is calculated

$$X_i = C_i \quad \text{..... (3)}$$

where C_i = mass concentration of element i (i = 1, ... x)

  - When the atomic concentration ratio is calculated

$$X_i = \frac{C_i}{A_i} \quad \text{..... (4)}$$

where A_i = Atomic weight of element i (i = 1, ... x)

- **In the case where the composition ratio as a compound is calculated, X_i in Equation (1) is expressed as follows.**

  - When the mass concentration ratio is calculated

    $$X_i = M_i \quad \text{..... (5)}$$

    where M_i = mass concentration of compound i (i = 1, ... x)
    M_i is calculated from the following equation.

    $$M_i = C_i \times \frac{A_i + R_i \times D}{A_i} \quad \text{..... (6)}$$

    where D = atomic weight of the coupling element
    R_i = Coupling ratio (i = 1, ... x)

  - When the molecular concentration ratio is calculated

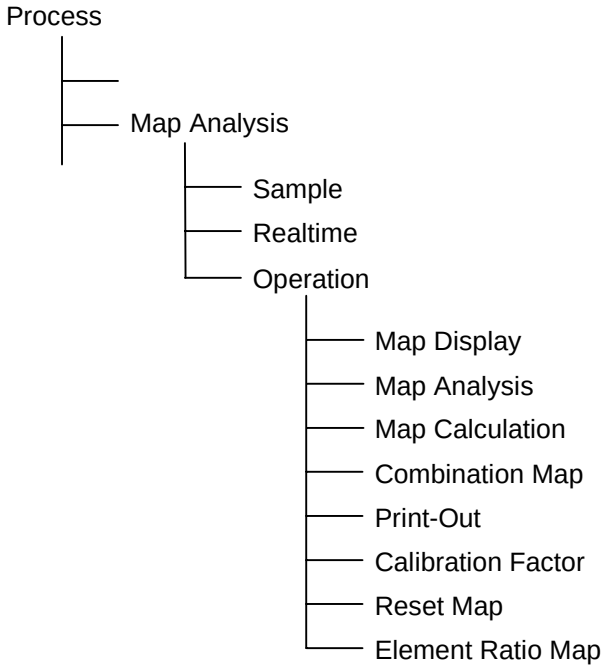
    $$X_i = \frac{N_i}{A_i + R_i \times D} \quad \text{..... (7)}$$

    where N_i = mass concentration of compound i (i = 1, ... x)

  As a special case, if all L_i in Equation (1) are 0, the denominator of Equation (1) will be treated as 1, and if the denominator of Equation (1) becomes 0 during the calculation process, M will be treated as 0.

2 PROGRAM COMPOSITION

This software consists of an Element Ratio Map in the Operation menu of the map analysis program.



3 OPERATION

This chapter assumes that map data which constitutes the base for element ratio map compilation has been acquired by the map analysis program.

3.1 Starting the Map Analysis Program

Click on the Process icon in the EPMA Menu, then select Map Analysis from the pull-down menu to start the program.

3.2 Displaying the Entry Map for Calculation

Click on the Sample button of the map analysis program to display the sample window, then select the Group name, Sample name, and map data, and display maps (entry maps) of specific components for compiling an element ratio map.
This program can handle maps of characteristic X-rays, backscattered electrons, secondary electrons, etc., for up to 15 components. At least one space has to be remained for displaying the result of mapping. In the example of Fig. 1, maps for three elements, Mg, Ca and Fe, have been selected. The specimen is a silicate mineral.

Entry maps can also be selected for different groups and different samples, however if the number of measuring points (number of x and y pixels) and the pixel size are different, meaningful results will not be obtained.

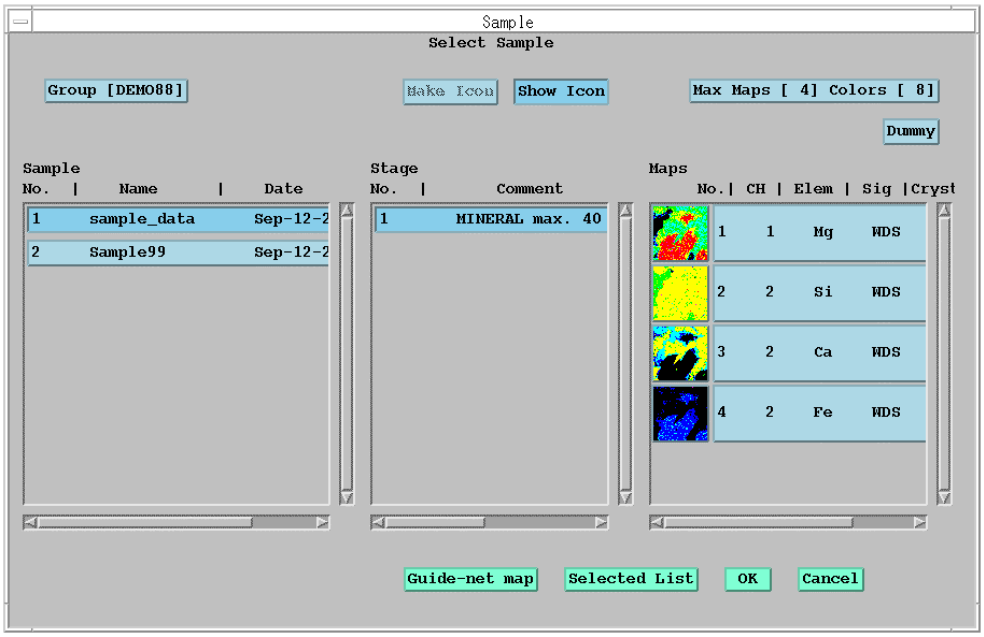


Fig. 1 Selecting the entry maps

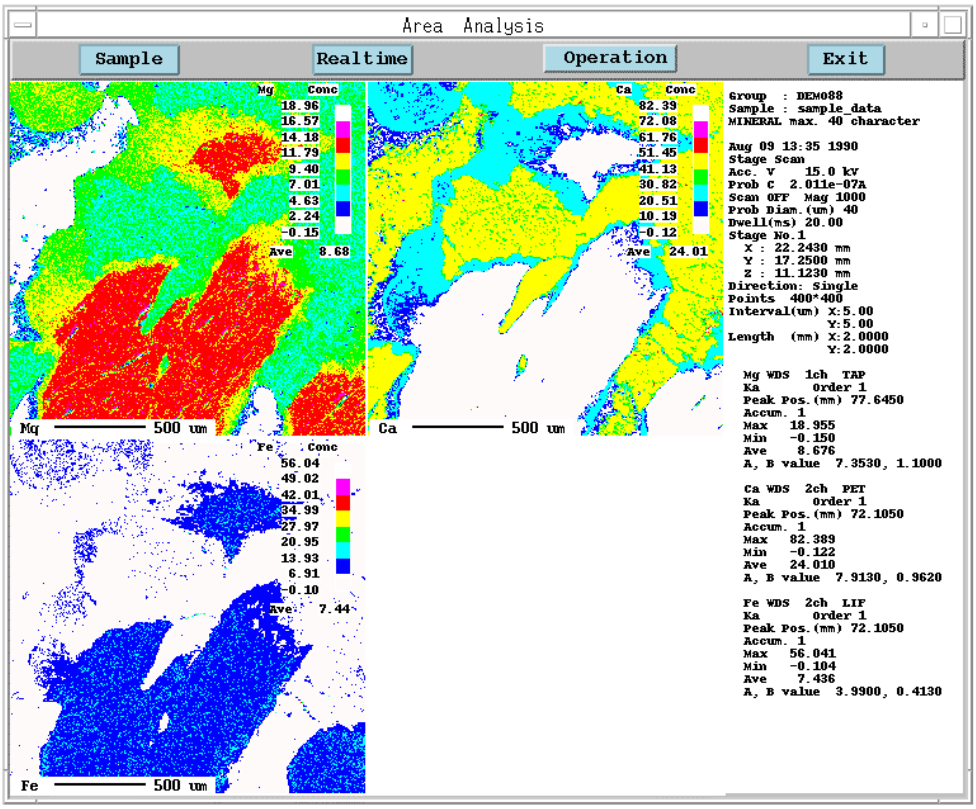


Fig. 2 Displaying the entry maps

3.3 Operation Window of the Element Ratio Map

If you click on the item “Element Ratio Map” (Fig. 3) in the Operation menu, the operation window of the element ratio map (see Element Ratio Map, Fig. 4) will appear. The signal names and element names corresponding to the entry maps will appear in this window.

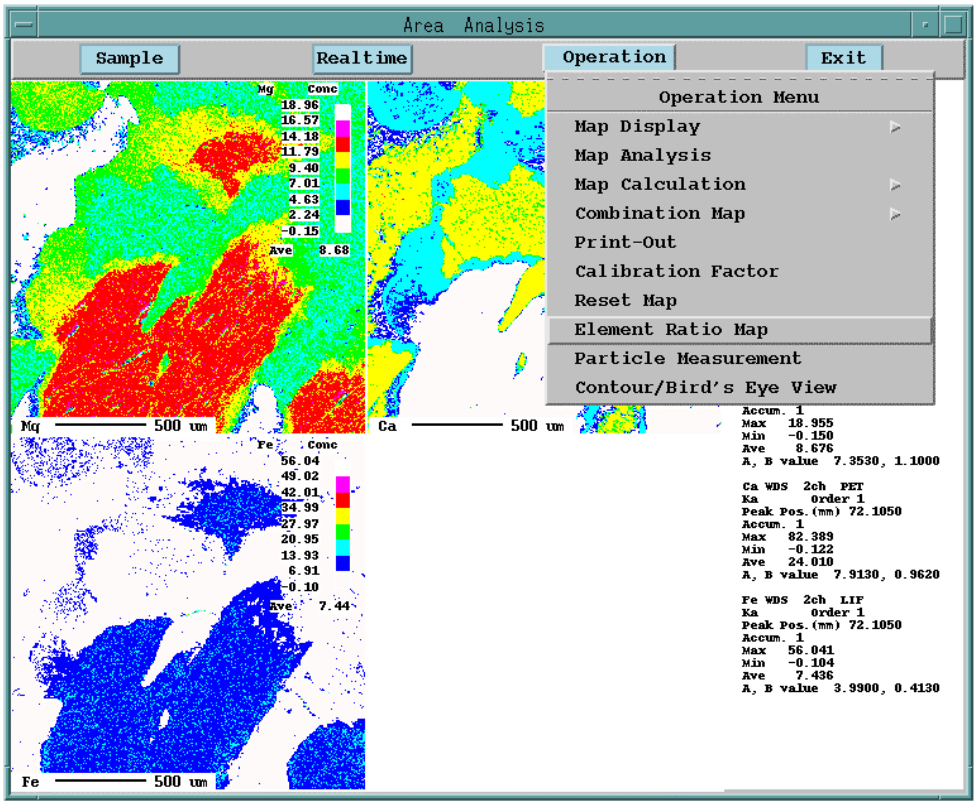
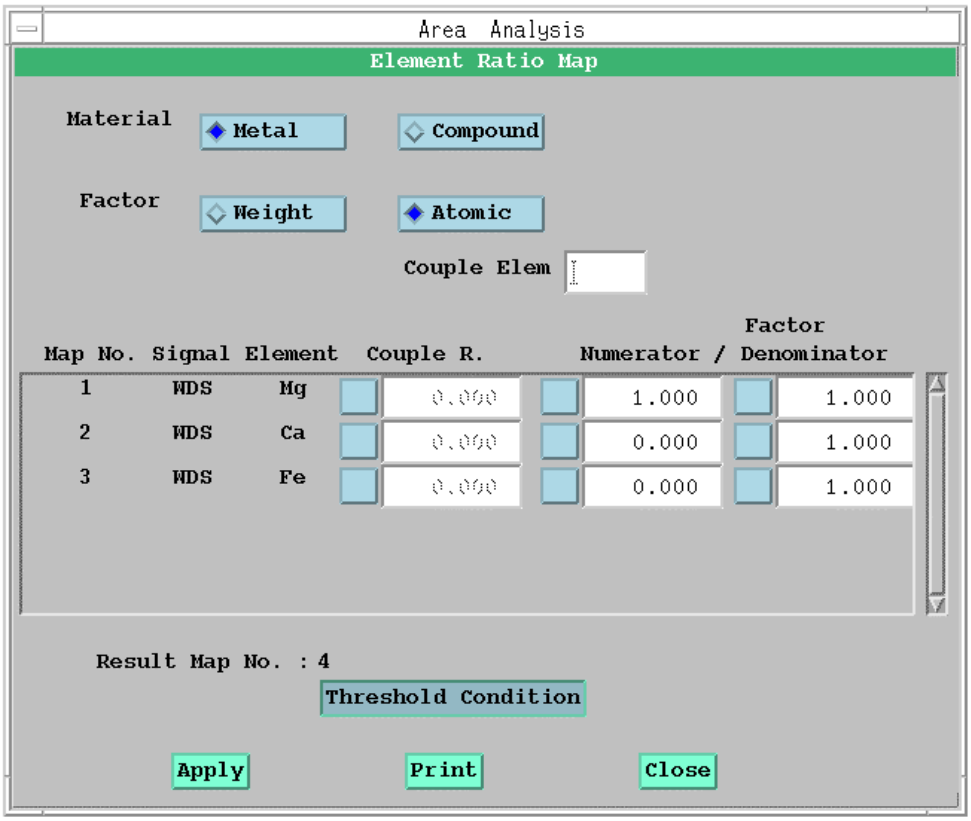


Fig. 3 Selecting the Element Ratio Map



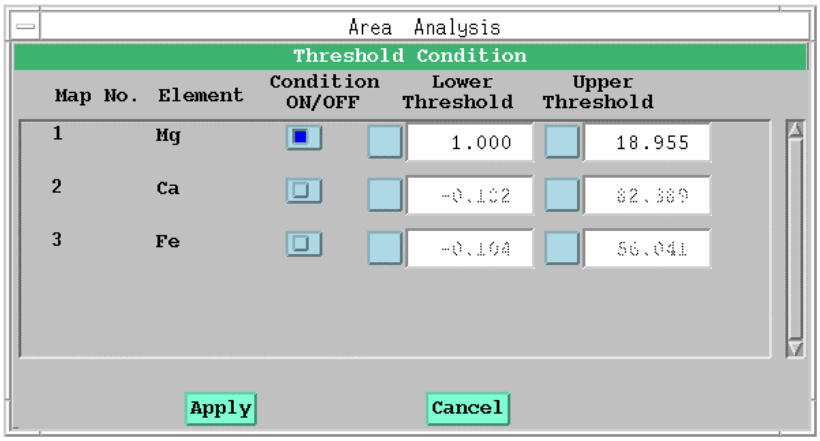


Fig. 4 Element Ratio Map window and Threshold Condition window

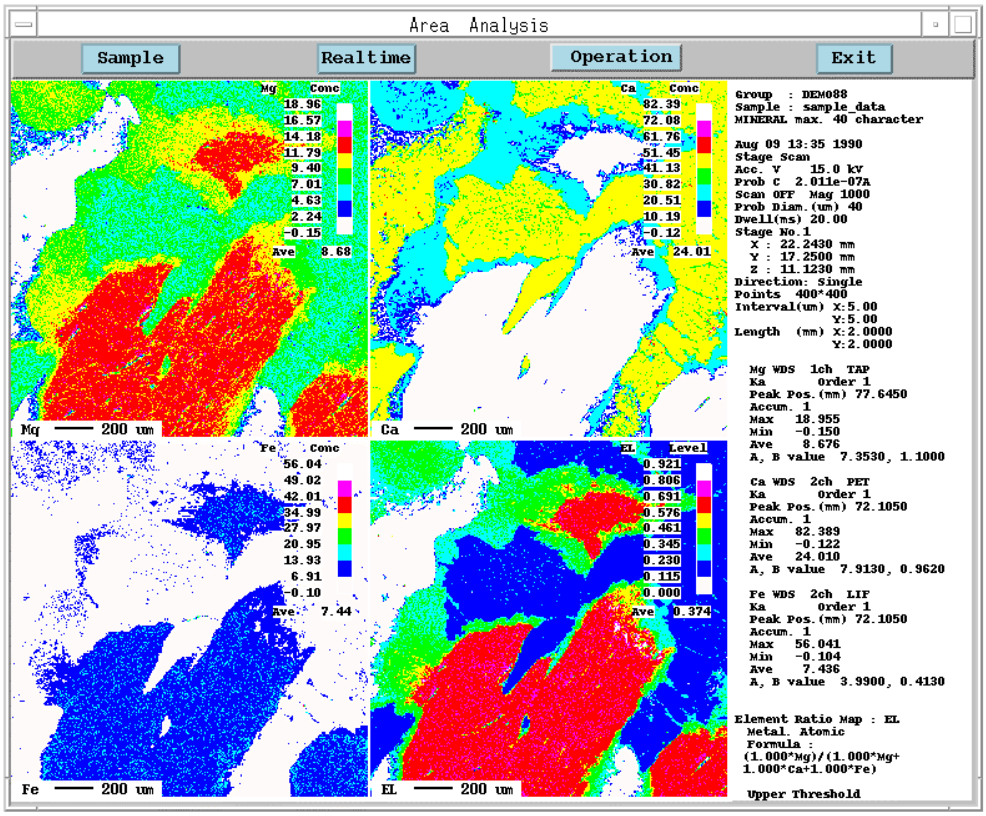


Fig. 5 Example of displaying the calculated results

If the entry maps (maps specified as the object of calculation) represent intensity, intensity will be displayed, while if they represent concentration, concentration will be displayed, and the element ratio map will be calculated. If both intensity and concentration are displayed, the message “Can’t calculate Element Ratio Map! ” will appear.

When calculating an element ratio map other than a simple intensity ratio, enter the conversion factor A and B values for intensity and concentration in advance, using “Calibration Factor” (calibration curve factor) in the Operation menu.

The map of the calculated results will be displayed at the position following the entry maps. If there is no space to display the result map, the message “No display space for the calculated map!” will appear. In this case, click on the OK button and increase Max Maps in the Sample window of Fig. 1 to a value that enables the maps including the calculated results to be displayed.

3.4 Entering the Calculation Conditions of the Element Ratio Map

Specify Metal or Compound for the item “Material” with the Element Ratio Map window of Fig. 4.

3.4.1 Metal

Select Metal for the item “Material”.

- **Mode**

  Weight or Atomic can be selected.

  - Weight: Calculates an element ratio map based on the mass concentration of the metal (single element). (☞ Refer to Equations (1) and (3) in “GENERAL”.)
  - Atomic: The element ratio map is compiled based on atomic concentration. (☞ Refer to Equations (1) and (4) in “GENERAL”.)

  ✍ In the case of Metal, an entry cannot be made to Couple Elem or Couple R.

  As a general rule, display the entry maps, using the metal element concentration values as the A and B values for the calibration curve in both the Weight and Atomic mode. If you use the A and B values for a compound in the calibration curve when using the Weight mode, the element ratio map of the mass concentration as a compound will be obtained. For map data of an image signal that has a name such as SL, CP, etc. that is not included in the atomic symbols, calculation takes place using an atomic weight of 1, for the sake of convenience.

3.4.2 Compound

If Compound is specified for the item “Material”, calculation will take place on the basis of a compound.

- **Mode**

  Select Weight or Molecule.

  - Weight: An element ratio map will be compiled as the mass concentration of a compound. (☞ Refer to Equations (1), (5) and (6) in “GENERAL”.) Display the entry maps, using the A and B values for a metal in the calibration curve.
  - Molecule: Compile an element ratio map as the molecular concentration. (☞ Refer to Equations (1) and (7) in “GENERAL”.) Use the values for a compound as the A and B values of the calibration curve.

- **Couple Elem**

  This is a coupling element. The default is O (oxygen). Enter an atomic symbol such as N, Cl, etc., or an atomic number. In addition to single elements, XO, OH, CO_2, SiO_2 and SO_3 can be entered. A coupling element does not need to be included in the map measurement elements.

- **Couple R. (coupling ratio)**

  This is equivalent to R of Equations (6) and (7) in “GENERAL”.

- **Numerator and Denominator**

  These are equivalent to Ki and Li, respectively, of Equation (1) in “GENERAL”.

- **Threshold Condition**

  You can set the upper and lower limits for element ratio calculation for each element. If you click on Threshold Condition button, the Threshold Condition window (☞ refer to Fig. 4) will appear. Here, click ON the Condition ON/OFF button for the element to be set, then enter values in Lower Threshold (LT) and Upper Threshold (UT).
  At points where the concentration (or intensity) of a specified element does not satisfy $LT \leq X \leq UT$, calculation will not be carried out, and the data corresponding to these points on the element ratio map will become 0.

- **Apply**

  Calculation will be carried out.

- **Print**

  You can print out the calculation conditions of an element ratio map by specifying the number of the displayed element ratio map in the Selection Map window, then by clicking on the Print button.

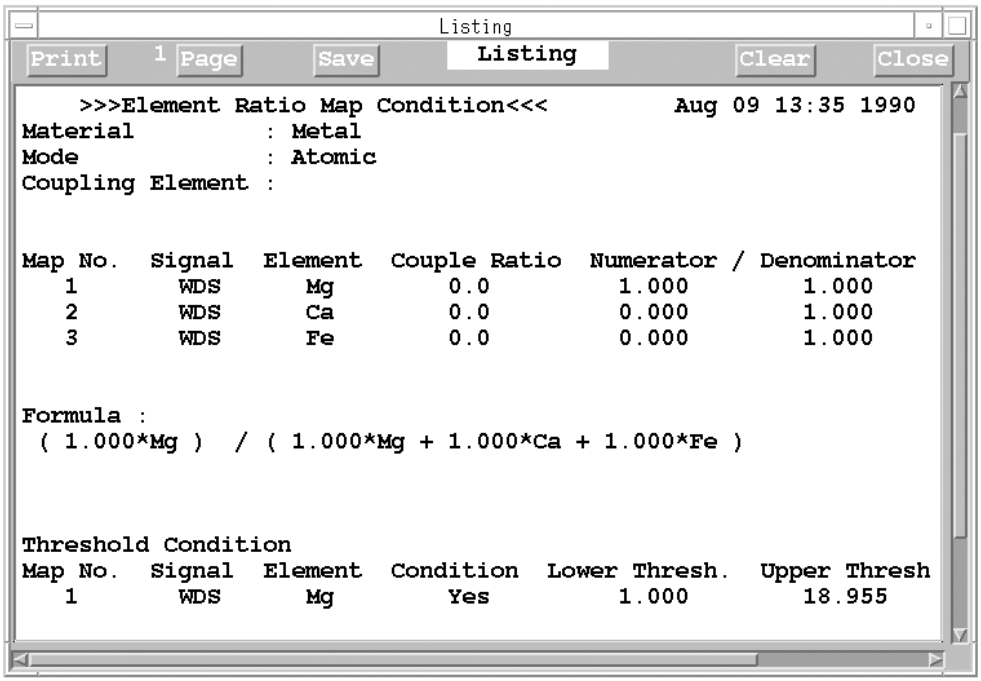


Fig. 6 Example of printout of an element ratio map

For reference

Example of specifying the Weight mode for Compound

If the coupling element for Si and Al is O, these elements are treated as SiO_2 and Al_2O_3, respectively. Here, if it is necessary to obtain the mass/concentration ratio of SiO_2 with respect to the mass concentration of these two oxides, select the Weight mode for Compound, then enter the following values.

Coupling ratio: 2 (= 2/1) and 1.5 (= 3/2), respectively

- Numerator: 1 and 0
- Denominator: 1 and 1

Use values for a metal as the A and B factors of the calibration curve of the entry map. (☞ Refer to Equations (1), (5) and (6) in "GENERAL".)
The value of Denominator for Al is 1 because the mass concentration of Al as the metal is multiplied by the ratio of the weight of $AlO_{1.5}$ and Al in Equation (6) to obtain the concentration of Al_2O_3 (= $AlO_{1.5}$).

Example of specifying the Molecule mode of Compound

If the coupling element for Mg, Al and Fe is O, these elements are treated as MgO, Al_2O_3 and Fe_3O_4, respectively. Here, if it is necessary to obtain the molecular concentration ratio of Al_2O_3 with respect to the molecular concentration of these three oxides, select Molecule mode for Compound, then enter the following values.

- Coupling ratio: 1 (= 1/1), 1.5 (= 3/2), and 1.333 (= 4/3)
- Numerator: 0, 0.5 (= 1/2), and 0
- Denominator: 1 (= 1/1), 0.5 (= 1/2), and 0.333 (= 1/3)

Use values for an oxide as the A and B values of the calibration curve of the entry map.

✍ The reasons for entering the above numerical values in each item are described below.

- Reason for entering 0, 0.5, and 0 in Numerator:
  With regard to Al, Al_2O_3 is considered to have twice the molecular weight of $AlO_{1.5}$, hence a correction factor of 1/2 should be used. The ratio for Al is to be calculated, so enter 0 for other elements.
- Reason for entering 1, 0.5, and 0.333 to Denominator:
  In the item "MgO", there is one MgO, hence a correction factor of 1 should be used. In the item "Al_2O", the molecular weight is twice that of $AlO_{1.5}$, hence a correction factor of 1/2 should be used. In the item "Fe_3O_4", the molecular weight is three times that of $FeO_{1.333}$, hence a correction factor of 1/3 should be used. (☞ Refer to Equations (1) and (7) of "GENERAL".)

The Threshold Condition window of Fig. 4 shows an example of an entry used to calculate the ratio of (the number of atoms of Mg)/(the total number of atoms of Mg, Ca and Fe), using a combination of Metal and Atomic.
The map at bottom right of Fig. 5 is the calculated result. The name EL is attached to the calculated data. EL is the default, however the name can be changed when saving the element ratio map. (☞ Refer to Sect. 3.5 "Storing an Element Ratio Map".)
The calculation conditions of this element ratio map can be displayed in the parameter display section of the screen. To display these conditions, set the item "Element Ratio" indicated by Display Parameter under Map Display of the Operation menu to ON.

3.5 Storing an Element Ratio Map

An element ratio map and its calculation conditions can be stored in a file or deleted. You can specify the map numbers for saving or deleting on the Selection Map window shown in Fig. 8. The elements ratio map can be saved using Result Store function after selecting the Map Calculation in the Operation menu in the Area Analysis window.

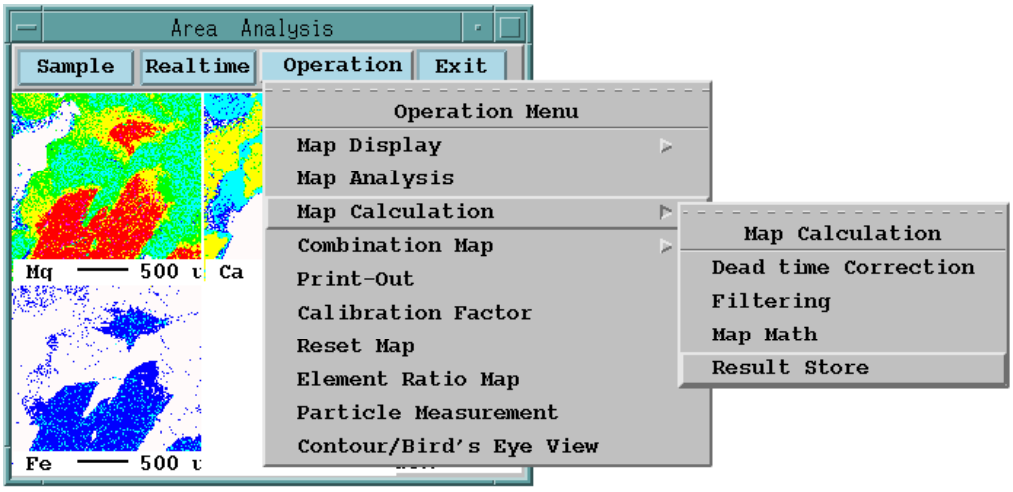


Fig. 7 Selecting the Map No. for storing an element ratio map

For example, enter EL in the Element box and CAL in the Crystal box and click the Save button. (See Fig. 8.)
To delete an element ratio map, click on the Delete button, or enter // in the Element box, and //////// in the Crystal box. As result, the file corresponding to the particular map number will be deleted.

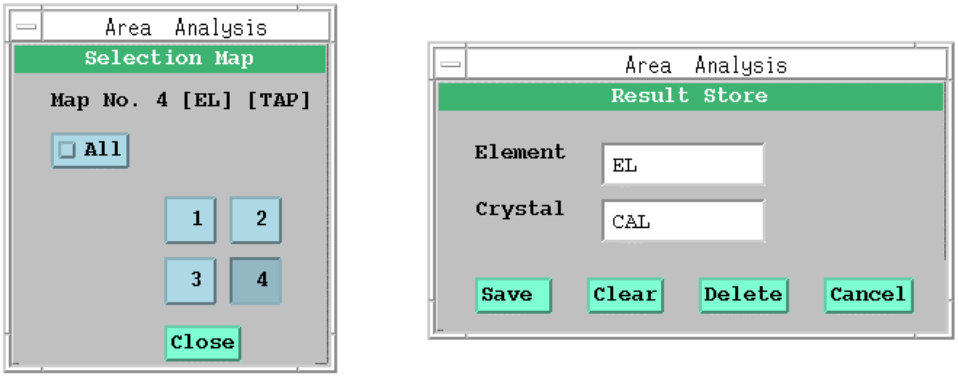


Fig. 8 Selection Map and Result Store windows