Hydrothermal/Accessory Minerals U-Th-Pb Data processing for LA-ICPMS

User Manual of Isoclock 2.0

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I. Software operation procedures

1.1 Start-up and functional block division

Windows users can also download and run the packaged exe file directly.

Download **Isoclock 2.0.exe:**

https://www.researchgate.net/publication/371012414_Isoclock20.

The demo video is available at:

https://www.researchgate.net/publication/371039144_Demo_of_Isoclock20.

The following steps 1.1.1-1.1.5 is run before Brama source code runs for the first time.

1.1.1 Python 3.9 is necessary to run the code. Download from https://www.python.org/downloads/ and follow the installation (Fig.1-1).

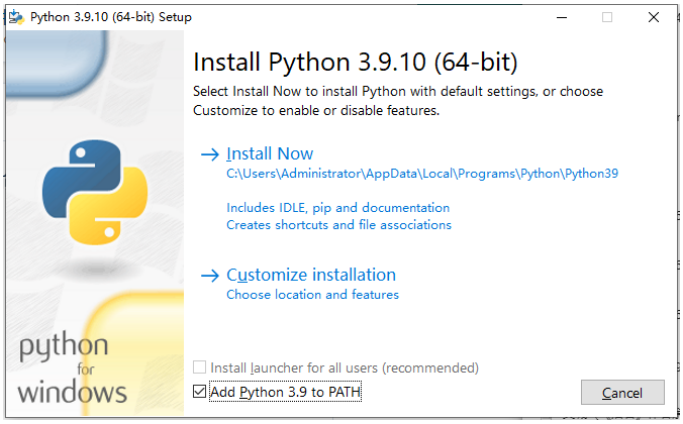

Fig. 1 Install Python 3.9.

1.1.2 Download or clone this repository（https://github.com/sndjgm/Isoclock）.

1.1.3 Open terminal/cmd and navigate to the Brama folder (Fig. 1-2).

- cd path/to/folder/ Isoclock

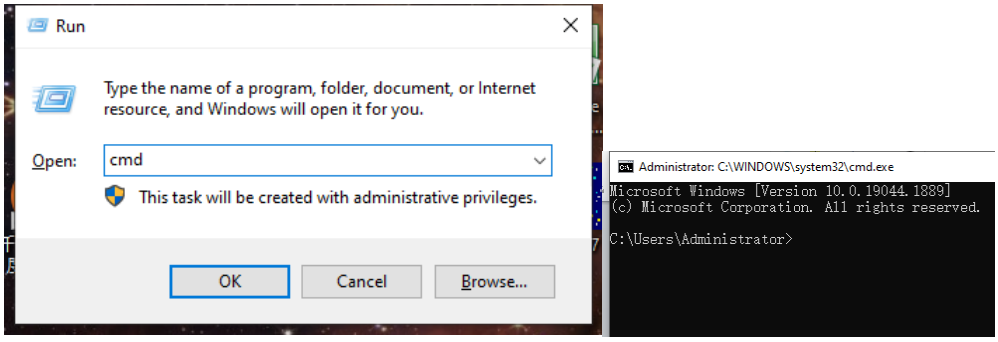

Fig. 2 Open terminal/cmd and navigate to the Isoclock folder.

1.1.4 Instal python libraries required for Isoclock.

- pip install -r requirements.txt.

1.1.5 Run Isoclock from python.

- python Isoclock.py

If everything is already installed, follow only steps1.1.5.

The main interface and functional partitions of the program are shown in Fig. 3 after starting.

Fig. 3 Main interface and function partition

The software is divided into 7 functional areas. The main functional areas are outlined as follows.

2. General steps of data processing:

The software interface is divided into different functional areas according to color (Fig. 3).

- ❖ (1) ~ (2) Select Mode.

Calculation mode selection area (light steel blue and dark blue): If the standards contain relatively high common Pb (such as apatite, sphere, wolframite, etc.) which needs to be corrected, select the <standard Cor> button. Otherwise, select <standard not Cor> button (e.g., for most zircon).

Dark blue area (2) switches the method of standard common Pb correction methods.

Common Pb correction method based on ^{207}Pb and ^{204}Pb derived from Chew et al. (2014). ^{208}Pb correction method derived from Zack et al.(2011).

(3) ~ (4) Set standard sample

Standard setting area (turquoise and grey): Click the <Setting Standard> button and select "S&k" mode （Stacey and Kramers, 1975）or "User" mode to set the standard information.

Note: when selecting the corresponding method directly, it is necessary to ensure that the standard sample name is completely consistent with the software display name.

❖ (5) Select ICPMS instrument model.

The software provides three formats to choose from:

(a) <**Thermo**> mass spectrometer. The software does not need to provide a “List file”(Excel with two columns of file serial number and sample name), and the software can automatically extract the document serial number and sample name;

(b) **<Agilent>** mass spectrometer. The file is stored in the 'sequence. CSV' file in the 'sequence. D' folder. It is necessary to provide the list format EXCEL file corresponding to the file sequence and sample name (the first column is the folder name, and the second column of the file is the sample or standard sample name);

(c) **<Element>** mass spectrometer. The "*. Fin" format file stores the list sequence file, and the "*. Fin2" format file stores the signal data.

❖ (6) Date input and output (light yellow):

Select the data input path and output path, and then click the <Load Data> button to import data. If <Agilent> is selected in step (3), the list file should be selected.Select the data input path and output path, and then click the < **Load Data** > button to import data.

Note: If **<Agilent>** is selected, you need to select the list file in the pop-up window.

❖ (7) Blank and sampling time settings (light purple):

Click the sample list on the left side of this area, and the signal diagram of the selected sample will be drawn in the area (10). Click the button <Set (All)> or < Set (Single)> to change the background and sampling time of selected or all signals.

❖ (8) Isotope ratio calculation (yellow-green):

Click <Fractionation Correction>button to generate the "result_all. csv" and “Mean_Cps.csv” file in the output directory.

❖ (9) Calculation of age results of samples (Saxe blue):

Click <Export (Liner)> to export the results of the calculated ages and isotope ratios of each sample with Sample-Standard-Bracketing method. No instrument drift correction is performed when the <Export (Average)> button is clicked.

The resulting file is named “cal_age_result_L*.xls” (Liner) or “cal_age_result_A*.xls” (average) (Fig. 4).

❖ (10) Signal diagram (white):

When the samples name in step (7) are selected, their signal diagram will be displayed here and automatically saved in the output directory.

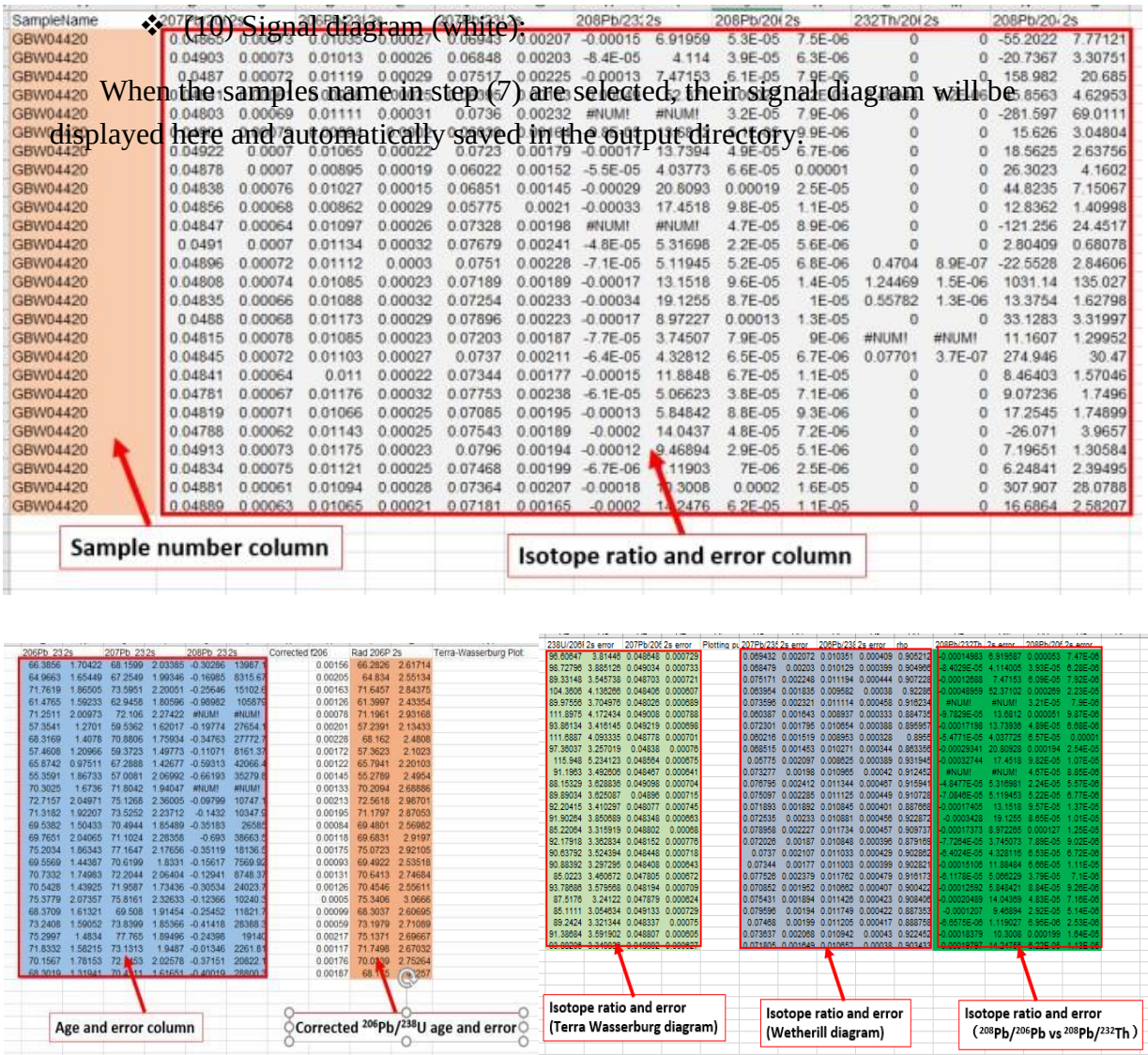

Fig. 4 description of software data processing results

Other Notes:

1. Input folder and output folder cannot be the same.
2. Only the original data is stored in the input folder, and there can be no other data files(such as CSV file of non-signal data), otherwise the program will report an error!
3. After processing one sample at a time, restart the program and replace with a new output folder directory.
4. Note that ^{204}Pb, ^{206}Pb, ^{207}Pb, ^{208}Pb, ^{232}Th and ^{238}U are required items, otherwise an error will be reported.
5. The first line of the “result_all.csv” file is the header, and the rest are in digital format.
6. When selecting the "Agilent" instrument, it is required to select the list file
7. when loading data. the first column is the folder name, the second column is the sample name, and the name of the list file worksheet must be "Sheet1".

Reference

Chew, D.M., Petrus, J.A., Kamber, B.S., 2014. U–Pb LA–ICPMS dating using accessory mineral standards with variable common Pb. Chemical Geology 363, 185-199.

Stacey, J.t., Kramers, J., 1975. Approximation of terrestrial lead isotope evolution by a two-stage model. Earth and Planetary Science Letters 26, 207-221.

Zack, T., Stockli, D.F., Luvizotto, G.L., Barth, M.G., Belousova, E., Wolfe, M.R., Hinton, R.W., 2011. In situ U–Pb rutile dating by LA-ICP-MS: 208Pb correction and prospects for geological applications. Contributions to Mineralogy and Petrology 162, 515-530.