

Computer program for the CHIME age calculation Takenori, KATO, Kazuhiro, SUZUKI and Mamoru ADACHI

**Department of Earth and Planetary Sciences, Graduate School of Science,
Nagoya University, Furo-cho, Chikusa-ku, Nagoya, 464-8602, Japan
(Received October 19, 1999 / Accepted November 11, 1999)*

ABSTRACT

A computer program for the CHIME age calculation is presented. By using reiteration procedures, the program saves significantly the time taken to estimate the isochron age from a dataset of ThO₂, UO₂ and PbO or Th, U and Pb analyses of Th- and/or U-bearing minerals. The program works under FreeBSD/i386 version 2.2.8 or later versions on IBM-PC and compatible computers and is available from <http://www.nendai.nagoya-u.ac.jp/gsd/CHIME/> through the Internet.

INTRODUCTION

The CHIME (Chemical Th-U-total Pb Isochron Method) dating method is based on the electron microprobe analysis of Th- and/or U-bearing minerals (Suzuki et al., 1991; Suzuki and Adachi, 1991a, b). The method offers a high spatial resolution and is applicable to subgrain dating of monazite, zircon, polycrase-euxenite, xenotime and allanite. Various studies using the CHIME method have been successful in revealing complex histories of orogenic belts (Suzuki et al., 1991; Suzuki and Adachi, 1991a, 1991b; Adachi and Suzuki, 1992; Adachi et al., 1992; Suzuki et al., 1992; Adachi and Suzuki, 1993; Enami et al., 1993; Morishita and Suzuki, 1993; Suzuki and Adachi, 1993; Adachi and Suzuki, 1994; Adachi et al., 1994; Suzuki and Adachi, 1994; Suzuki et al., 1994; Suzuki et al., 1994; Adachi and Suzuki, 1995; Khan et al., 1995; Morishita and Suzuki 1995; Suzuki et al., 1995; Asami et al., 1996; Cho et al., 1996; Nakai and Suzuki, 1996; Suzuki et al., 1996; Suzuki et al., 1996; Suzuki et al., 1996; Asami et al., 1997; Ito et al., 1997; Kato et al., 1997; Kim et al., 1997; Tadesse et al., 1997; Asami et al., 1998; Bindu et al., 1998; Chang et al., 1998; Suzuki and Adachi, 1998; Suzuki et al., 1998;). Recently, the chemical Th-U-total Pb dating using an electron microprobe has been done by many authors in addition to the originator's group (Montel et al., 1996; Rhede et al., 1996; Cocherie et al., 1998; Braun et al., 1998; Williams et al., 1999).

Although conventional chemical Th-U-total Pb dating methods do not provide information about discordancy in the Th-U-Pb system, the CHIME method has the advantage of lead loss detection and common lead estimation by means of an isochron method. However, the calculation of isochron from the data set of EPMA Th, U and Pb analysis is not easy without computer programs, because the system contain three different decay chains. The original CHIME age calculation program runs on only NEC PC-9801 series and its compatible computers. Therefore, it is hard to use the program for many geoscientists in the world. We here present an alternative com-

puter program to calculate CHIME ages for IBM-PC and compatible computers. This paper introduces the outline of the computer program and compares its results with that from the originators' program.

THE CHIME AGE CALCULATION

Details of the CHIME age calculation have been reported in Suzuki and Adachi (1991a, 1991b, 1994). From the concentrations of U, Th and Pb, apparent age t is calculated from:

$$\frac{\text{PbO}}{\text{W}_{\text{Pb}}} = \frac{\text{ThO}_2}{\text{W}_{\text{Th}}} \{ \exp(\lambda_{232} t) - 1 \} + \frac{\text{UO}_2}{\text{W}_{\text{U}}} \left\{ \frac{\exp(\lambda_{235} t) + 137.88 \exp(\lambda_{238} t)}{138.88} - 1 \right\} \quad (1)$$

where

PbO: concentration of PbO

ThO₂: concentration of ThO₂

UO₂: concentration of UO₂

W_{Pb}: molecular weight of Pb (= 224 for ThO₂-rich minerals and = 222 for UO₂-rich minerals),

W_{Th}: molecular weight of Th (= 264)

W_U: molecular weight of U (= 270)

λ_{232} : decay constants (= $4.9475 \times 10^{-11}/\text{y}$, Steiger and Jäger, 1977)

λ_{235} : decay constants (= $9.8485 \times 10^{-10}/\text{y}$, Steiger and Jäger, 1977)

λ_{238} : decay constants (= $1.55125 \times 10^{-10}/\text{y}$, Steiger and Jäger, 1977)

In the calculation for ThO₂-rich mineral, the apparent amount of total ThO₂ (ThO₂^{*}) is given by:

$$\text{ThO}_2^* = \text{ThO}_2 + \frac{\text{UO}_2 \cdot \text{W}_{\text{Th}}}{\text{W}_{\text{U}} \{ \exp(\lambda_{232} t) - 1 \}} \cdot \left\{ \frac{\exp(\lambda_{232} t) + 137.88 \exp(\lambda_{238} t)}{138.88} - 1 \right\} \quad (2)$$

and in a calculation for UO₂-rich mineral, the apparent amount of total UO₂ (UO₂^{*}) is given by:

$$\text{UO}_2^* = \text{UO}_2 + \frac{138.88 \text{ThO}_2 \cdot \text{W}_{\text{U}} \{ \exp(\lambda_{232} t) - 1 \}}{\text{W}_{\text{Th}} \{ \exp(\lambda_{235} t) + 137.88 \exp(\lambda_{238} t) - 138.88 \}} \quad (3)$$

The relationship between PbO and ThO₂^{*} or PbO and UO₂^{*} values are given by:

$$\begin{cases} \text{PbO} = m \cdot \text{ThO}_2^* + b & (\text{ThO}_2\text{-rich mineral}) \\ \text{PbO} = m \cdot \text{UO}_2^* + b & (\text{UO}_2\text{-rich mineral}) \end{cases} \quad (4)$$

where m is a function of T . Isochron procedure gives estimated values for m and

b and estimated ages and the amount of initial PbO can be calculated from them. Recalculation of ThO₂* or UO₂* with estimated T and isochron procedure provide revised estimates. Reiteration of this procedure provides reliable estimate of age and initial PbO.

COMPUTER PROGRAM

The computer program described in this paper performs reiteration of the isochron procedure described above. Isochron procedure is based on York (1966).

The computer program is available from <http://www.nendai.nagoya-u.ac.jp/gsd/CHIME/> through the Internet. The binary file for FreeBSD/i386 2.2.8 and later versions is provided.

(Comparison with the originators' program)

Even though we consider that the present program in this paper is reliable, we compare its results with that by the originators' program. Published EPMA analysis of monazite and zircon grains (Suzuki and Adachi, 1994) are used in this comparison (Table 1). For the monazite grain, the program in this paper gives:

$$253 \pm 24 \text{ Ma (MSWD} = 0.16)$$

and the originators' program gives:

$$253 \pm 24 \text{ Ma (MSWD} = 0.17)$$

For zircons grain, the program in this paper gives:

$$2036 \pm 58 \text{ Ma (MSWD} = 0.07)$$

and the originators' program gives:

$$2036 \pm 57 \text{ Ma (MSWD} = 0.07)$$

These calculations clearly indicate that the results by the present program conforms to that by the originators' program.

(File Format)

A file read by the program is a text file. Each line has following seven fields:

```

'Spot ID':String for identification
ThO2: ThO2 in wt.%
error of ThO2:relative analytical error of ThO2 in %
UO2: UO2 in wt.%
error of UO2:relative analytical error of UO2 in wt.%
PbO: PbO in wt.%
error of PbO:relative analytical error of PbO in wt.%

```

Table 1: Analytical data of monazite and zircon grains from the Hida gneiss on Oki-Dogo Island (taken from Suzuki and Adachi 1994)

Spot ID	ThO ₂ wt.%	error %	UO ₂ wt.%	error %	PbO wt.%	error %
Monazite grain M71 from sample 0304						
M71-01	7.25	1	0.832	5	0.106	5
M71-02	6.88	1	0.672	5	0.092	10
M71-03	6.69	1	0.349	5	0.085	10
M71-04	6.79	1	1.41	2	0.123	5
M71-05	7.02	1	0.458	5	0.089	10
M71-06	7.21	1	1.13	2	0.115	5
M71-07	7.92	1	0.560	5	0.108	5
M71-08	7.08	1	0.405	5	0.087	10
M71-09	7.11	1	0.668	5	0.098	10
M71-10	7.80	1	1.499	2	0.132	5
M71-11	7.77	1	1.816	2	0.146	5
M71-12	7.28	1	1.299	2	0.122	5
M71-13	6.80	1	0.929	5	0.100	5
M71-14	7.14	1	0.447	2	0.092	10
Zircon grain Z209 from sample 0304						
Z209-1	0.083	10	0.186	10	0.069	10
Z209-2	0.155	10	0.187	10	0.077	10
Z209-3	0.181	10	0.314	5	0.119	5
Z209-4	0.302	5	0.392	5	0.159	5
Z209-5	0.143	10	0.112	10	0.050	10
Z209-6	0.188	10	0.321	5	0.121	5
Z209-7	0.093	10	0.163	5	0.060	10
Z209-8	0.544	5	0.399	5	0.186	5

The spot ID field should not contain white space (space and tab). Each field should be separated by white spaces like:

M01-01 2.20 1.1 0.228 3.8 0.069 14.6

No comment line should be in a file.

The above example shows that (1) spot ID is 'M01-01', (2) ThO₂ = 2.20 wt.% and its relative analytical error is 1.1%, (3) UO₂ = 0.228 wt.% and its relative analytical error is 3.8% and (4) PbO = 0.069 wt.% and its relative analytical error is 14.6%. If command line option '-m' is set (see below), it shows that (1) spot ID is 'M01-01', (2) Th = 2.20 wt.% and its relative analytical error is 1.1%, (3) U = 0.228 wt.% and its relative ana-

tical error is 3.8% and (4) Pb = 0.069 wt.% and its relative analytical error is 14.6%.

(Command line options)

The program has following command line options:

- u UO₂-rich mineral mode. Use this option when you calculate the CHIME age of UO₂-rich mineral (e.g. zircon).
- t ThO₂-rich mineral mode. Use this option when you calculate the CHIME age of ThO₂-rich mineral (e.g. monazite).
- v displays analysis results, apparent ages and RO*2 for each spot.
- f file tells file for input. If this option is not specified, the program read data from standard input.
- m assumes that concentrations are amounts of metals instead of oxides. Default is oxide-mode.

One of -u and -t options is mandatory. When the option '-m' is specified, amounts of PbO, ThO₂ and UO₂ are calculated by

$$\text{PbO} = \begin{cases} \text{PbO} \cdot \frac{224}{208} & (\text{ThO}_2\text{-mineral mode}) \\ \text{PbO} \cdot \frac{222}{206} & (\text{UO}_2\text{-mineral mode}) \end{cases} \quad (5)$$

$$\text{ThO}_2 = \text{Th} \cdot \frac{264}{232}$$

$$\text{UO}_2 = \text{U} \cdot \frac{270}{238}$$

When the EPMA analysis of zircon is stored in the file 'zircon', typing

```
chime -u -f zircon
```

gives the CHIME age, error and MSWD (Fig. 1). When the EPMA analysis of monazite is stored in the file 'monazite' typing

```
chime -vt -f monazite
```

gives the CHIME age, error, MSWD and spot ID, concentrations and analytical error

```
% chime -u -f zircon
Number of data point: 8          MSWD=0.071520
  Age / Ma = 2035.680177    +/-    58.355947
inclination = 0.341159    +/-    0.012659
intercept = -0.002484    +/-    0.003832
```

Fig. 1: Calculation result using the present program for the zircon.

```

% chime-vt-fmonazite
Number of datapoint:14          MSWD=0.157437
  Age /Ma = 253.156361 +/- 23.731568
inclination = 0.010694 +/- 0.001009
  intercept = -0.000901 +/- 0.010499

SpotNo. ThO2   Error UO2   Error PbO   Error Age  RO2*
M71-01  7.2500  1.0  0.8320  5.0  0.1060  5.0  252  9.9482
M71-02  6.8800  1.0  0.6720  5.0  0.0920  10.0  241  9.0593
M71-03  6.6900  1.0  0.3490  5.0  0.0850  10.0  257  7.8218
M71-04  6.7900  1.0  1.4100  2.0  0.1230  5.0  256  11.3626
M71-05  7.0200  1.0  0.4580  5.0  0.0890  10.0  248  8.5053
M71-06  7.2100  1.0  1.1300  2.0  0.1150  5.0  250  10.8746
M71-07  7.9200  1.0  0.5600  5.0  0.1080  5.0  263  9.7361
M71-08  7.0800  1.0  0.4050  5.0  0.0870  10.0  245  8.3934
M71-09  7.1100  1.0  0.6680  5.0  0.0980  10.0  250  9.2763
M71-10  7.8000  1.0  1.4990  2.0  0.1320  5.0  247  12.6613
M71-11  7.7700  1.0  1.8160  2.0  0.1460  5.0  253  13.6593
M71-12  7.2800  1.0  1.2990  2.0  0.1220  5.0  251  11.4927
M71-13  6.8000  1.0  0.9290  5.0  0.1000  5.0  241  9.8127
M71-14  7.1400  1.0  0.4470  2.0  0.0920  10.0  254  8.5896

```

Fig. 2: Calculation result using the present program for the monazite. Spot ID, concentrations and analytical errors of oxide, apparent age and amount of total oxide (RO₂*) of each spot are also shown since '-v' option is specified.

of oxides, apparent age and ThO*₂ or UO*₂ for each spot (Fig. 2).

ACKNOWLEDGMENTS

Dr. R. Metralfe of Tono Geoscience Center of Japan Nuclear Cycle Development Institute reviewed the manuscript and provided constructive comments.

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