



(U-Th)/He dating: principles and applications

Cécile Gautheron

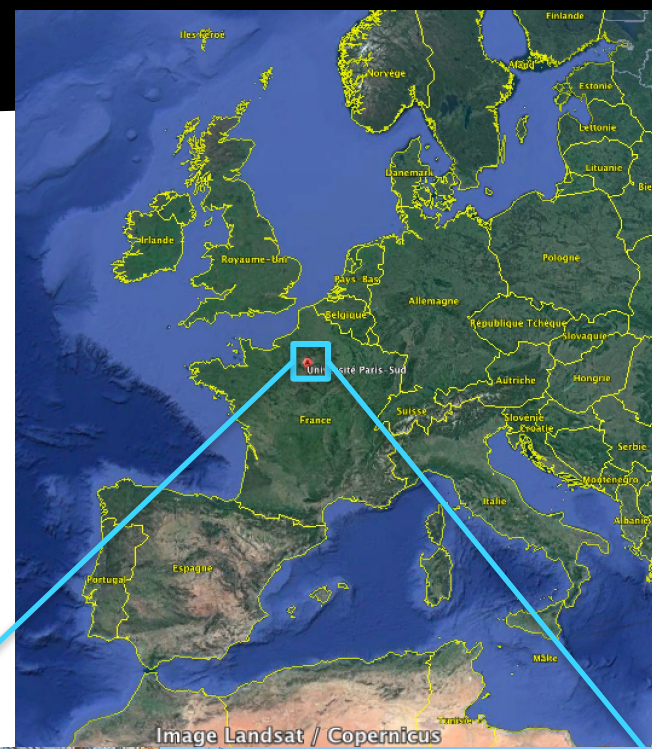
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Helsinki University – 26 octobre 2017

Paris universities

University of Paris Notre Dame (Sorbonne)
was born in 1150 (2nd university in Europe)

=> Introduced several academic standards
such as doctoral degrees



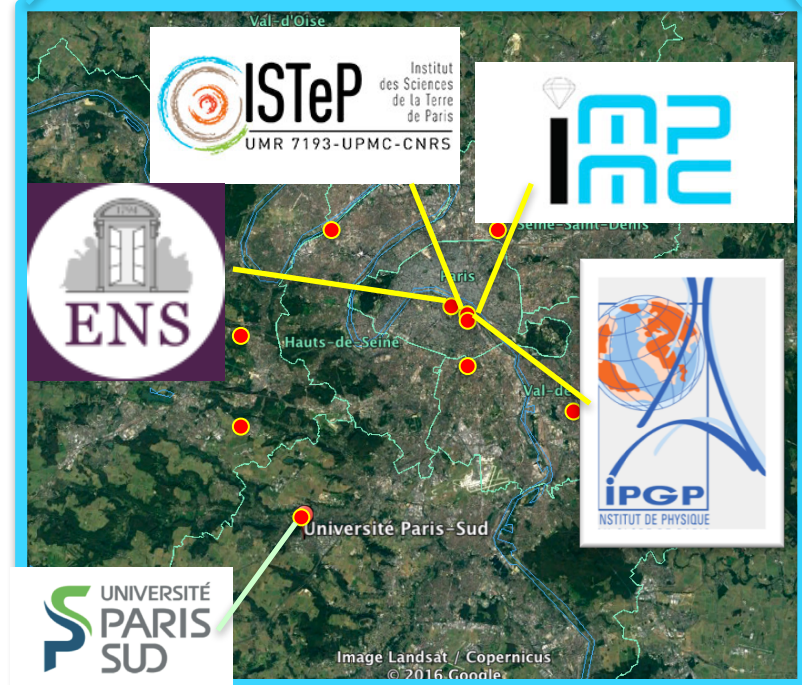
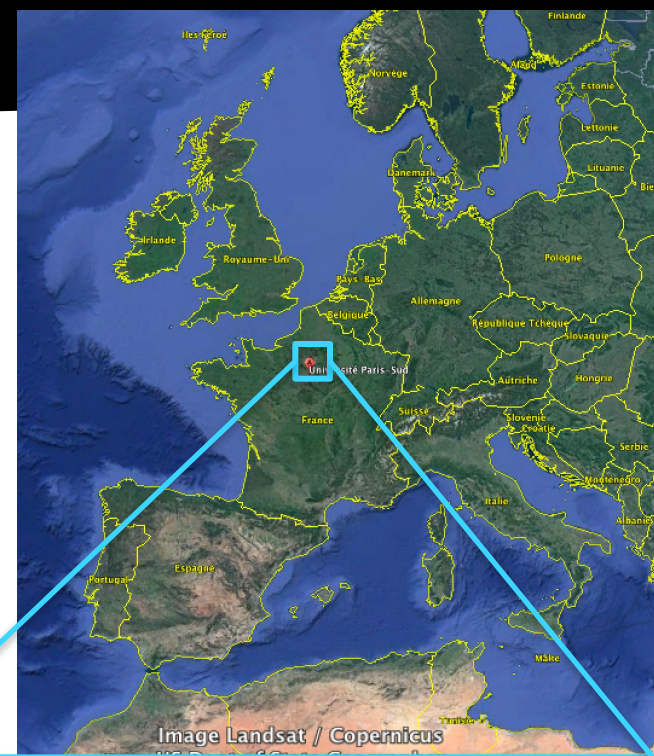
Paris universities

After 1968 => 15 autonomous universities

More than 7 universities with a Geosciences department

University Paris Sud 11 was born in 1955

- 30 000 students from 125 nationalities
- 2500 researchers (40 in the Earth Science department)
- Pluridisciplinary research



(1) (U-Th)/He dating system

I. Introduction, generalities

II. (U-Th)/He principles (chronometer vs thermochronometer)

(2) How to get an (U-Th)/He age

(3) Applications

III. Apatite (U-Th-Sm)/He (AHe) method

IV. Other applications (zircon, iron oxides,...)

(4) Exercises (Tc, ejection, weight, Rs), thermal modeling

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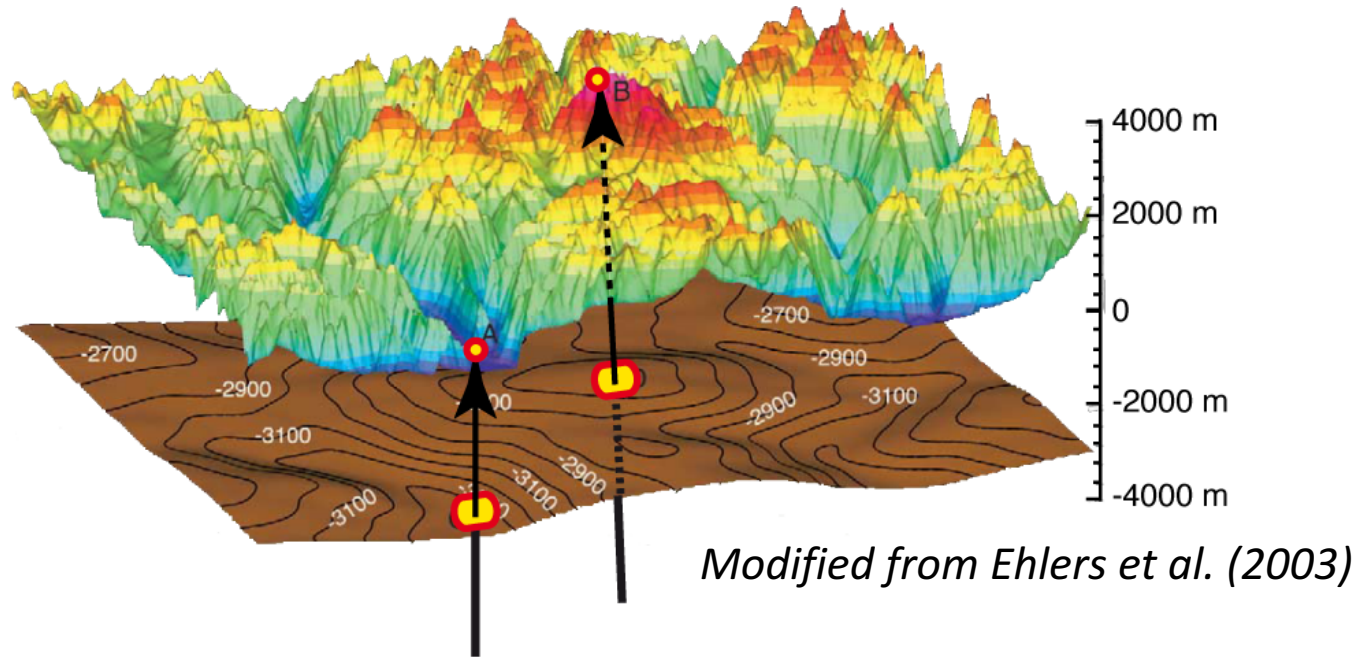
(3) Applications

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I. Quantification of rocks thermal evolution through time

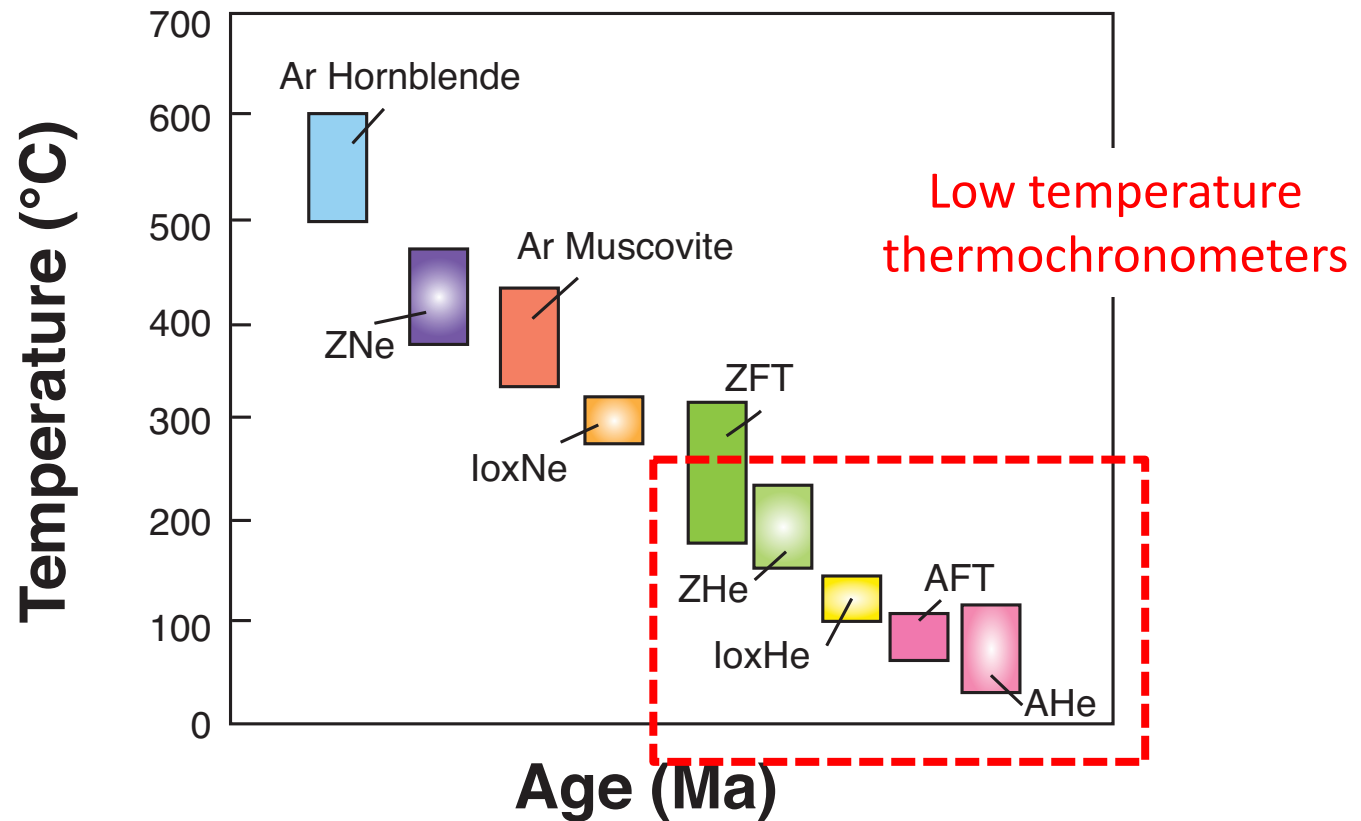


U-Th-Sm (parent) => He (daughter)

Complete daughter retention => **chronometer**

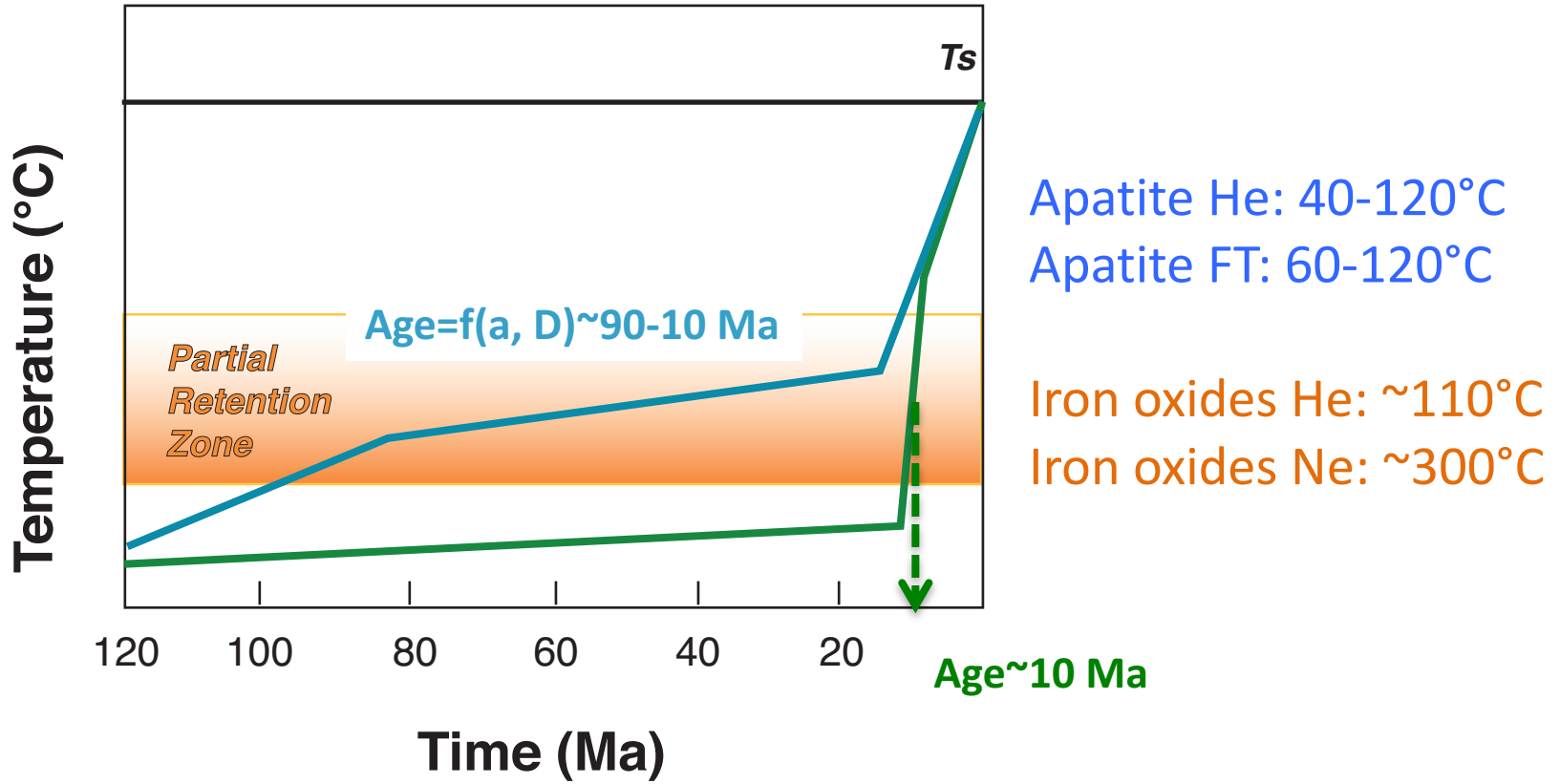
Daughter loss by diffusion => **thermochronometer**
(Closure temperature and Partial Retention Zone)

I. Thermal sensitivity of thermochronometers



- **(U-Th)/⁴He** method applied on apatite, zircon and iron oxides
- Thermal sensitivity from 40 to 200°C

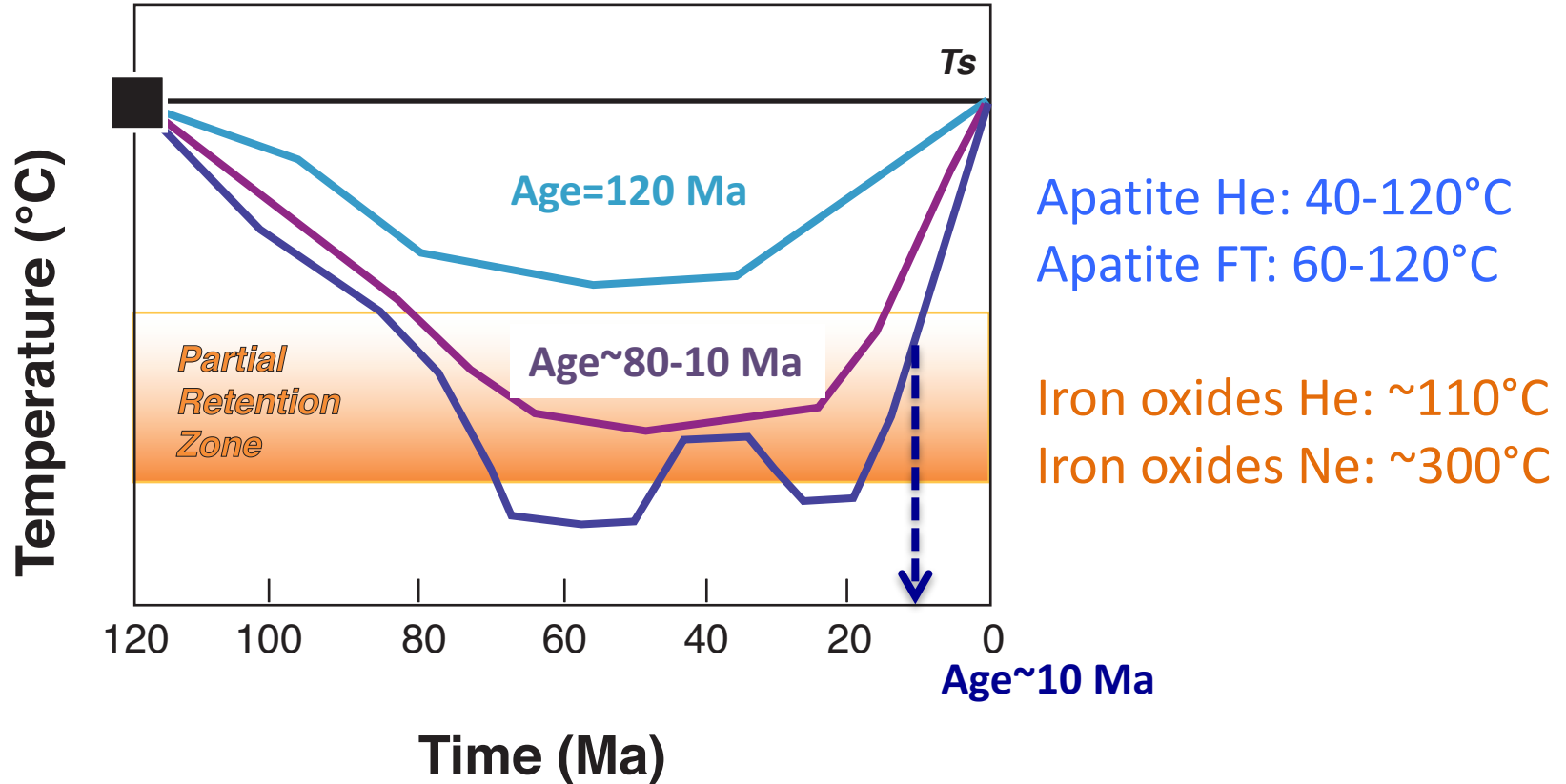
I. Meaning of thermochronological ages



Plutonic rock example:

Rock formation age > thermochronometric age

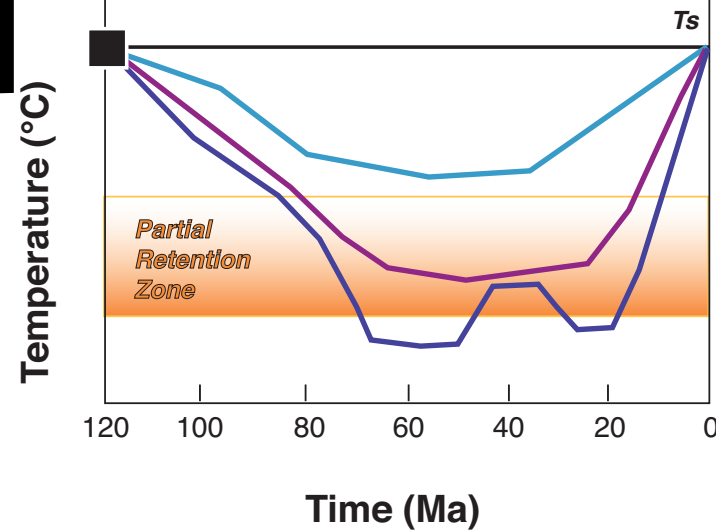
I. Meaning of thermochronological ages



Sedimentary, volcanic rock or iron oxides duricrust examples:

Rock formation age \geq or \leq thermochronometric age

I. Meaning of thermochronological ages



TAKE HOME MESSAGE:

- A thermochronological age (or date) is an **apparent** age
- Need to apply some **corrections** (alpha ejection, diffusion)
- ^4He accumulation in crystal lattice reflects = **f (thermal history, diffusion coefficient, grain size, ...)**

I. Quantification of erosion and weathering processes

- **Apatite, zircon, titanite...** can be used to quantify **rock thermal history** and **erosion processes ...**



- **Iron oxides (hematite, goethite)** can be used to quantify **weathering episodes** (paleosurfaces), **timing of ore deposits ...**

(1) (U-Th)/He dating system

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(3) Applications

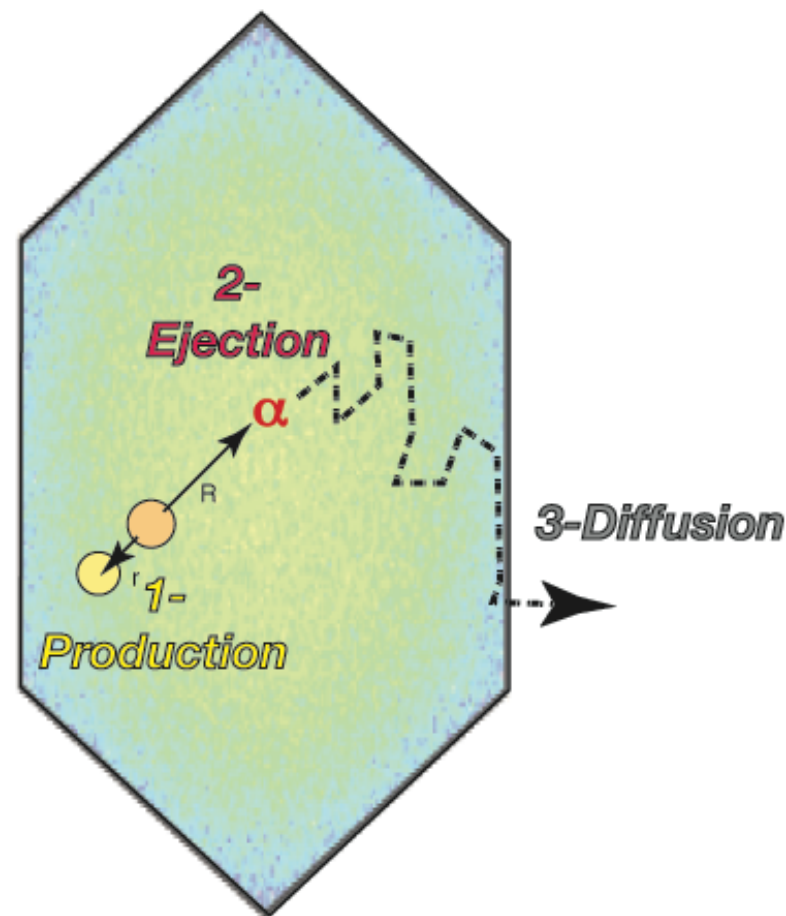
III. Apatite (U-Th-Sm)/He (AHe) method

IV. Other applications (zircon, iron oxides,...)

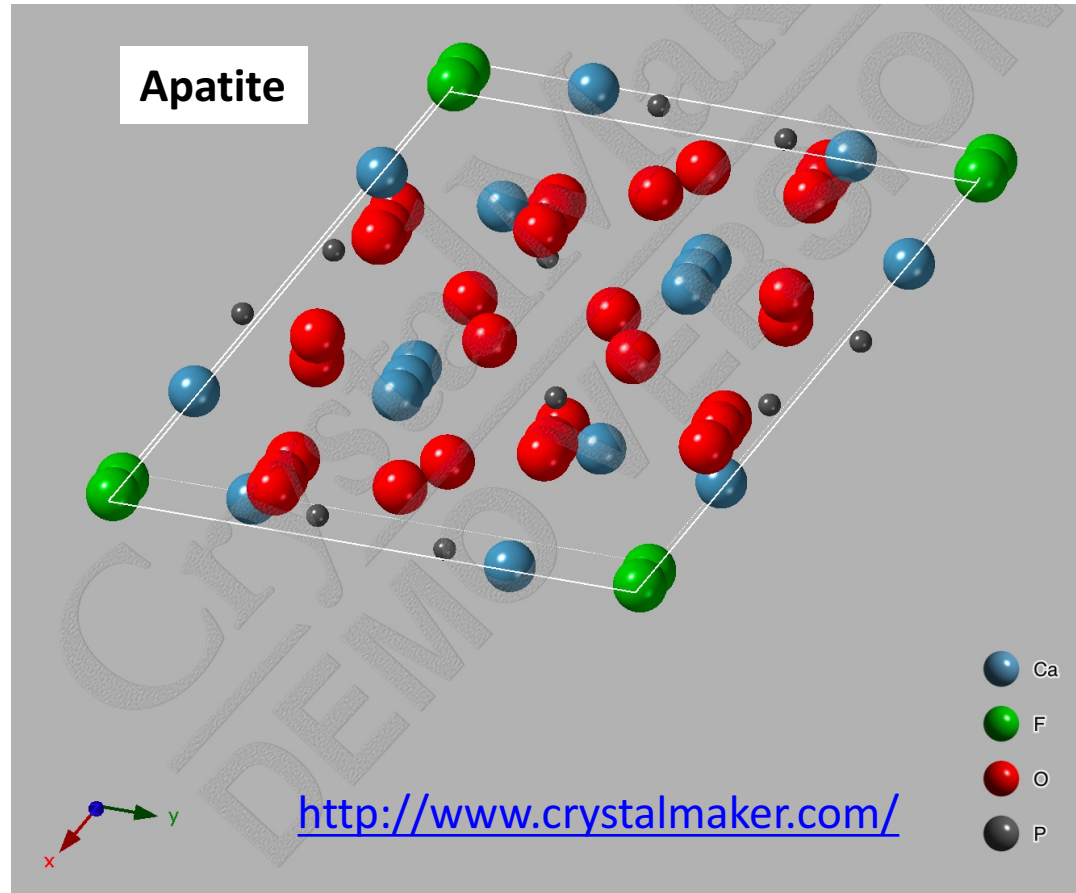
(4) Exercises (Tc, ejection, weight, Rs), thermal modeling

II. (U-Th-Sm)/He dating method principles

- 1) He atoms production in minerals during U, Th, Sm decay
- 2) Long alpha ejection (15-20 μm)
- 3) Possible diffusion in the crystal, depending on :
 - a) diffusion coefficients and
 - b) thermal history



II. U-Th-Sm incorporation in crystal lattice

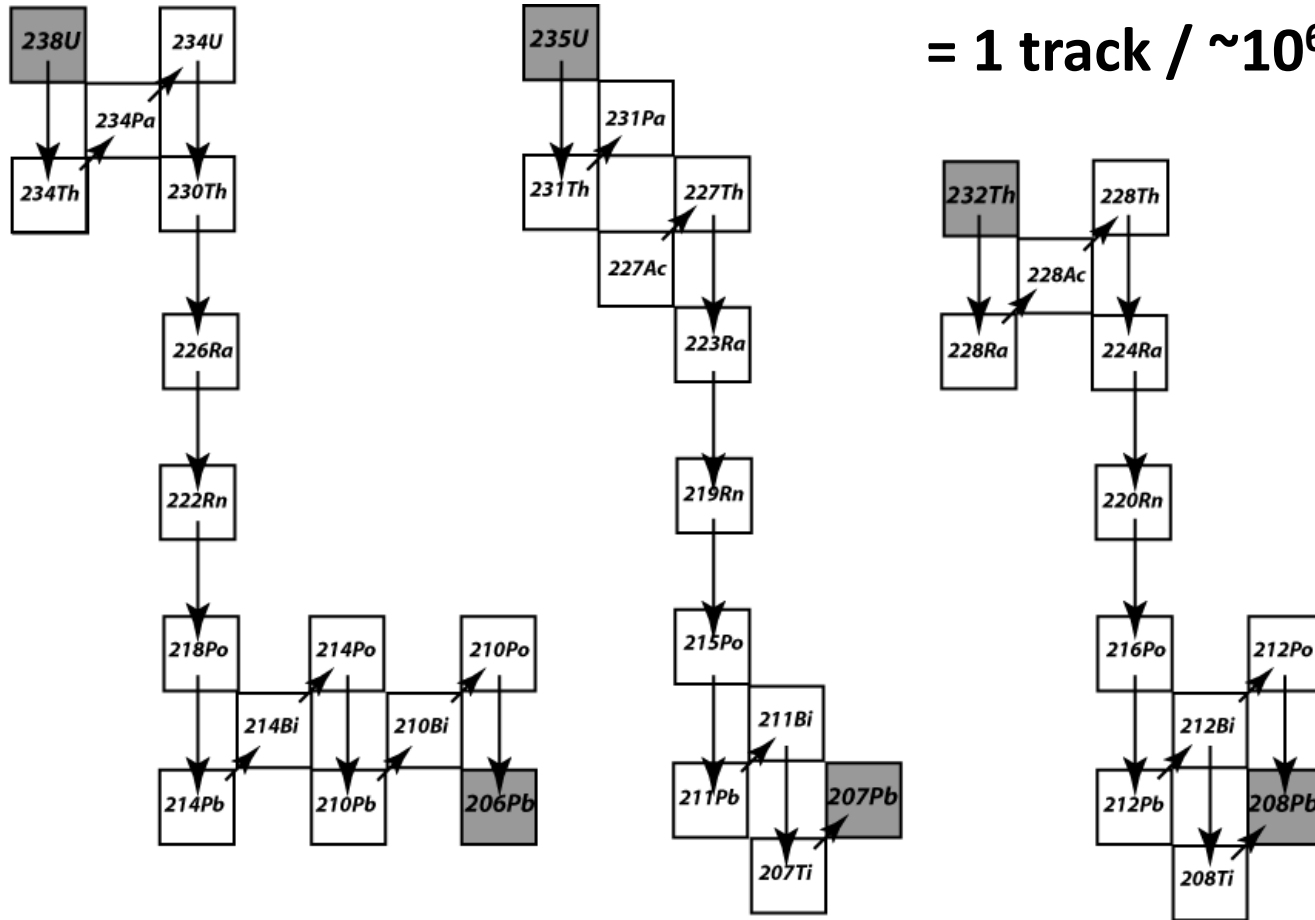


U, Th and Sm incorporation (substitution or cluster) in almost any crystal lattice:

➤ **U** = 0.01 - 1000 ppm; **Th/U** = 0.1 - 20; **Sm** = 10 - 3000 ppm

II. U-Th-Sm radioactive natural decay

U
Pa
Th
Ac
Ra
Fr
Rn
At
Po
Bi
Pb
Ti

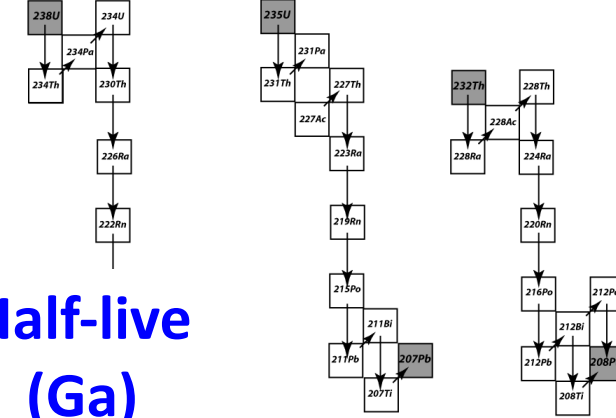


^{238}U natural fission
= 1 track / $\sim 10^6$ alphas

➤ $^{235}\text{U} + ^{238}\text{U} = 99.99\% \text{ U}$; $^{232}\text{Th} = 100\% \text{ Th}$ and $^{147}\text{Sm} = 0.15\% \text{ Sm}$

II. U-Th-Sm radioactive natural decay

U
Pa
Th
Ac
Ra
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Rn
At

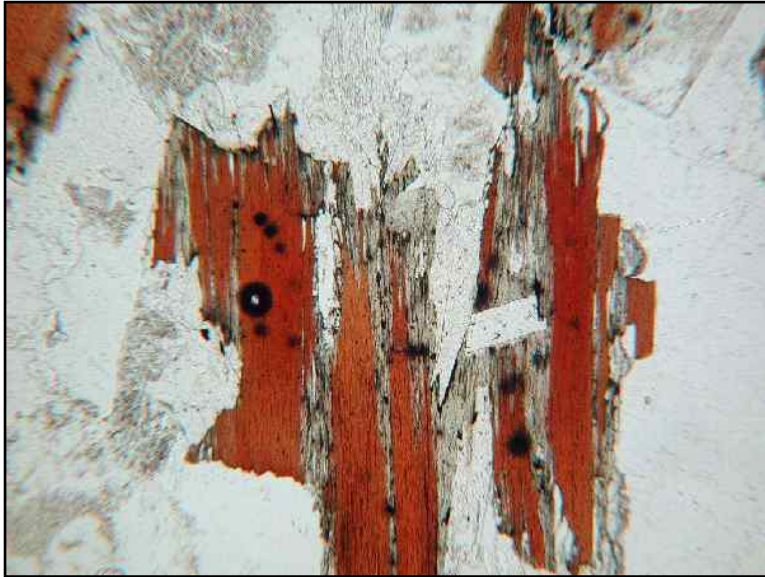


Father	Daughter	Nb. α particles	Half-life (Ga)
^{238}U	^{206}Pb	+ 8 α	(4.4683)
^{235}U	^{207}Pb	+ 7 α	(0.7038)
^{232}Th	^{208}Pb	+ 6 α	(14.05)
^{147}Sm	^{143}Nd	+ 1 α	(106)

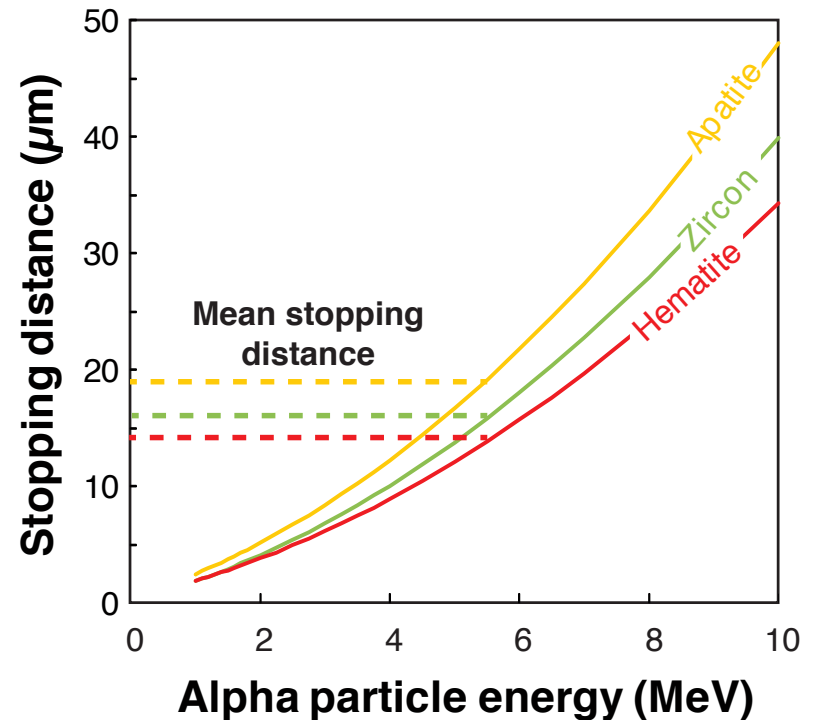
➤ Alpha particles production during U-Th-Sm alpha decay

II. Alpha particles production => high energies

SRIM; Ziegler (2008); Ketcham et al. (2011)



Alpha halo in biotite



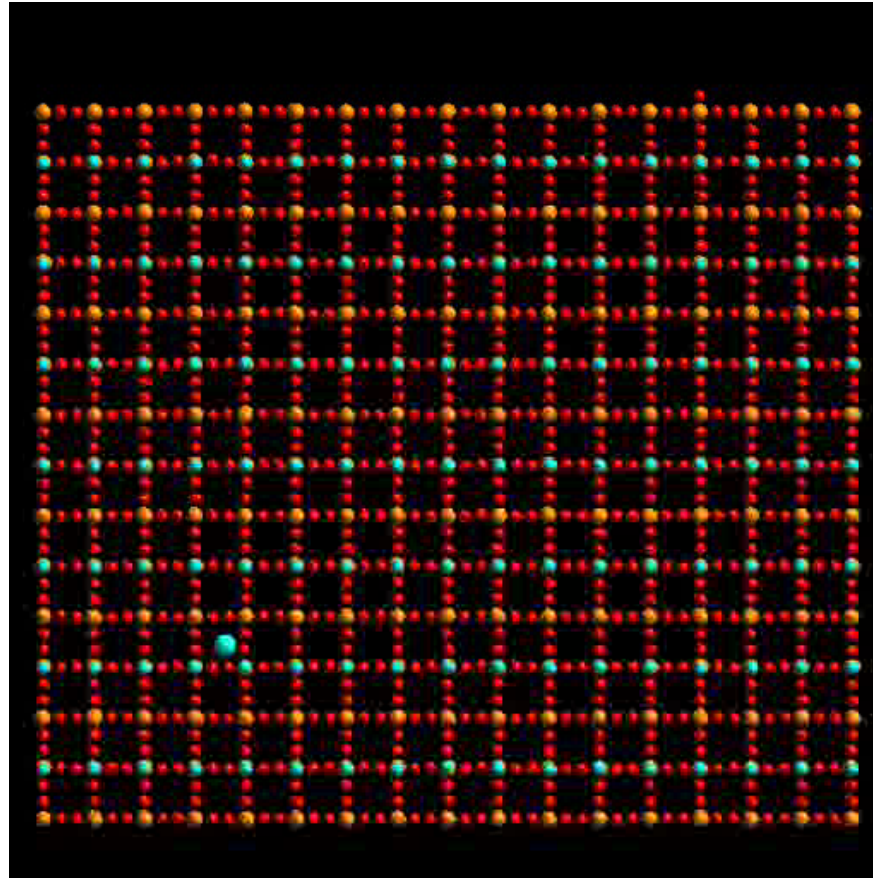
High kinetic energy of α particles,

α -----> ^4He (after taking electrons)

He atoms will stop after some microns depending on initial energy, lattice density, chemistry and Th/U ratio (See EXERCICE 1).

II. Alpha particles energies = recoil damage

Trachenko, 2003



Associated to alpha decays, the “father” element will do a recoil.

➤ **Damage creation at nanometer scale**

II. ${}^4\text{He}$ production

$$[\text{He}] =$$

$$\left(8 \times \frac{137.88}{138.88} \left(e^{\lambda_{238}t} - 1 \right) + 7 \times \frac{1}{138.88} \left(e^{\lambda_{235}t} - 1 \right) \right) \times [U]$$

From ${}^{238}\text{U}$
and ${}^{235}\text{U}$

$$+ \left(6 \times \left(e^{\lambda_{232}t} - 1 \right) \right) \times [\text{Th}]$$

From
 ${}^{232}\text{Th}$

$$+ \left(1 \times 0.1499 \times \left(e^{\lambda_{147}t} - 1 \right) \right) \times [\text{Sm}]$$

From
 ${}^{147}\text{Sm}$

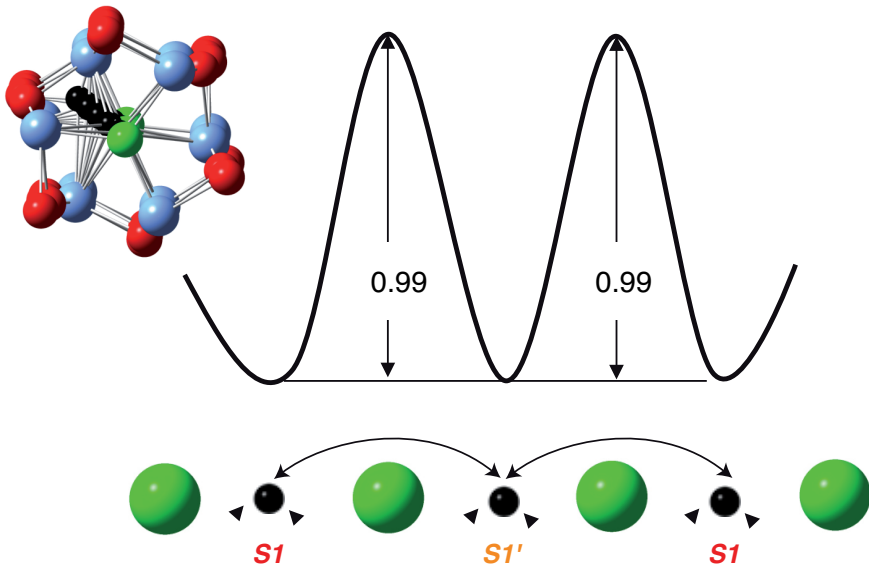
➤ **eU (effective Uranium) = U + 0.24 Th + 0.0005 Sm**

II. Diffusion in minerals : microscopic or macroscopic point of view

Diffusion is a microscopic (atomic) process that can be seen :

Microscopic level :

1D

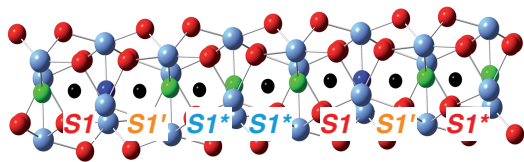


II. Diffusion in minerals : microscopic or macroscopic point of view

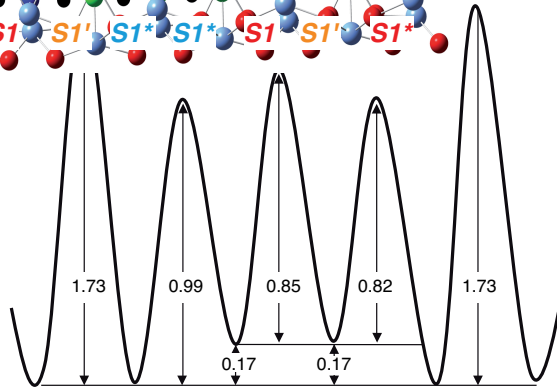
Diffusion is a microscopic (atomic) process that can be seen :

Microscopic level :

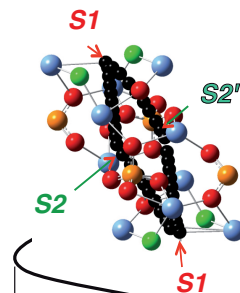
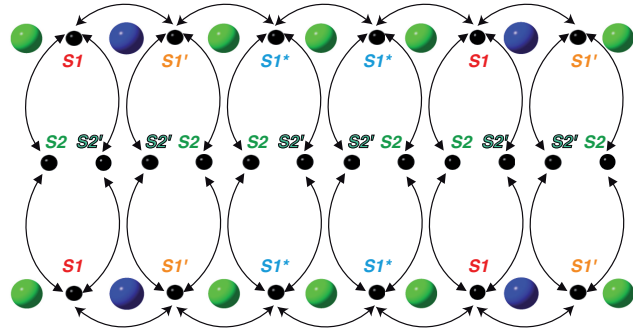
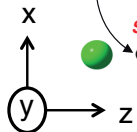
2D



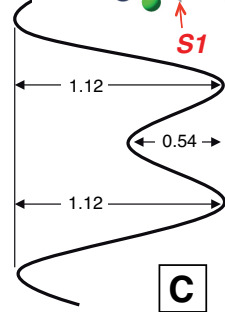
B



A

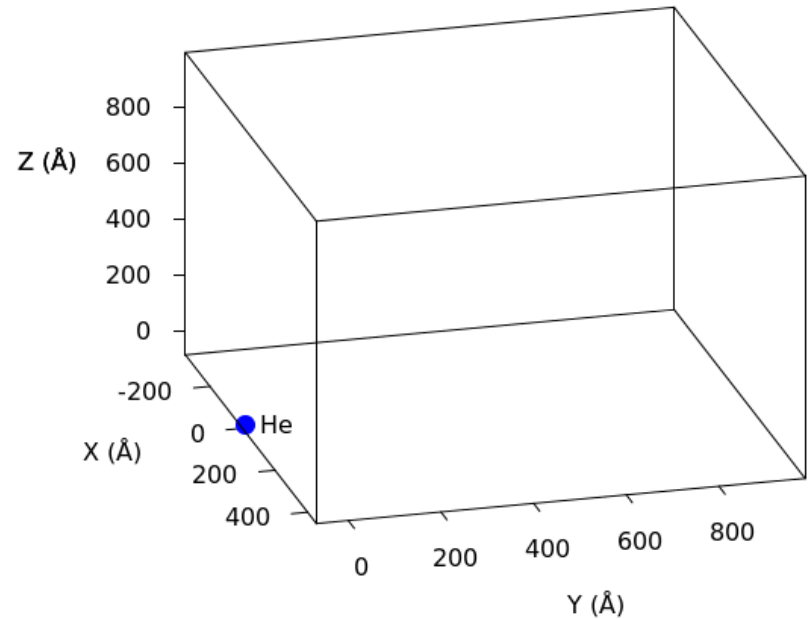


C



3D

t = 0.00765516 Sec.



Balout et al. (2017)

Djimbi et al. (2015)

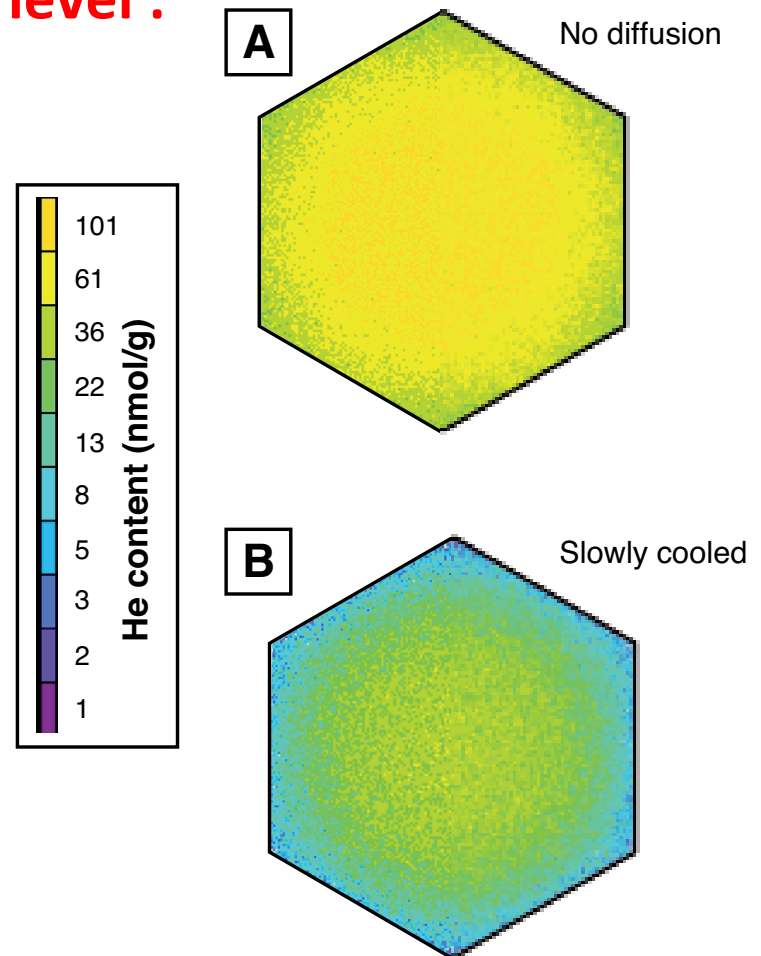
II. Diffusion in minerals : microscopic or macroscopic point of view

Diffusion is a microscopic (atomic) process that can be seen :

Macroscopic level :

✧ Random diffusion can be described at macroscopic level using Fick's law:

$$\frac{\partial C}{\partial t} = D \left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2} \right)$$



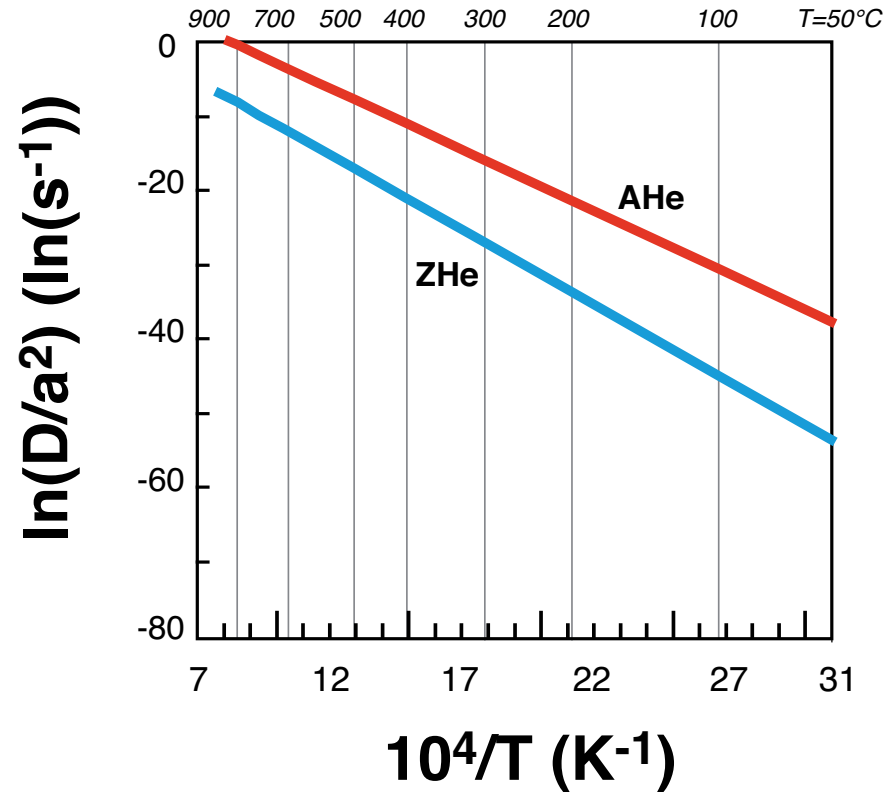
II. Diffusion coefficient in minerals

At first order, diffusion coefficient, D , follows the Arrhenius law:

$$\frac{D}{a^2} = \frac{D_0}{a^2} \exp\left(\frac{-E_a}{RT}\right)$$

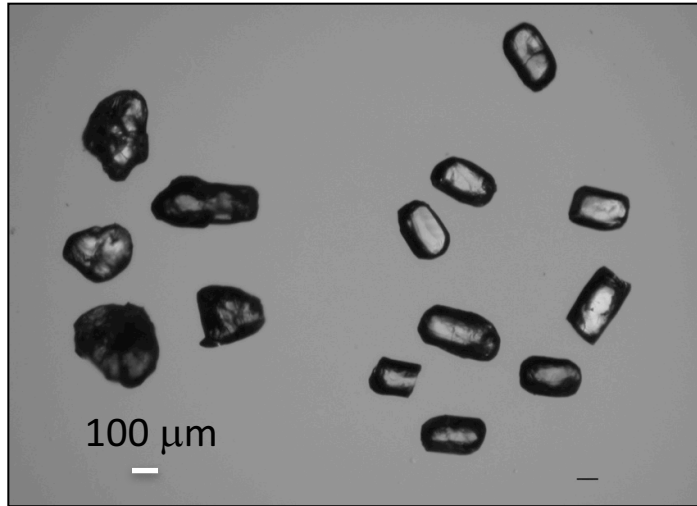
One unique D_0 and E_a

Different size (a) domains

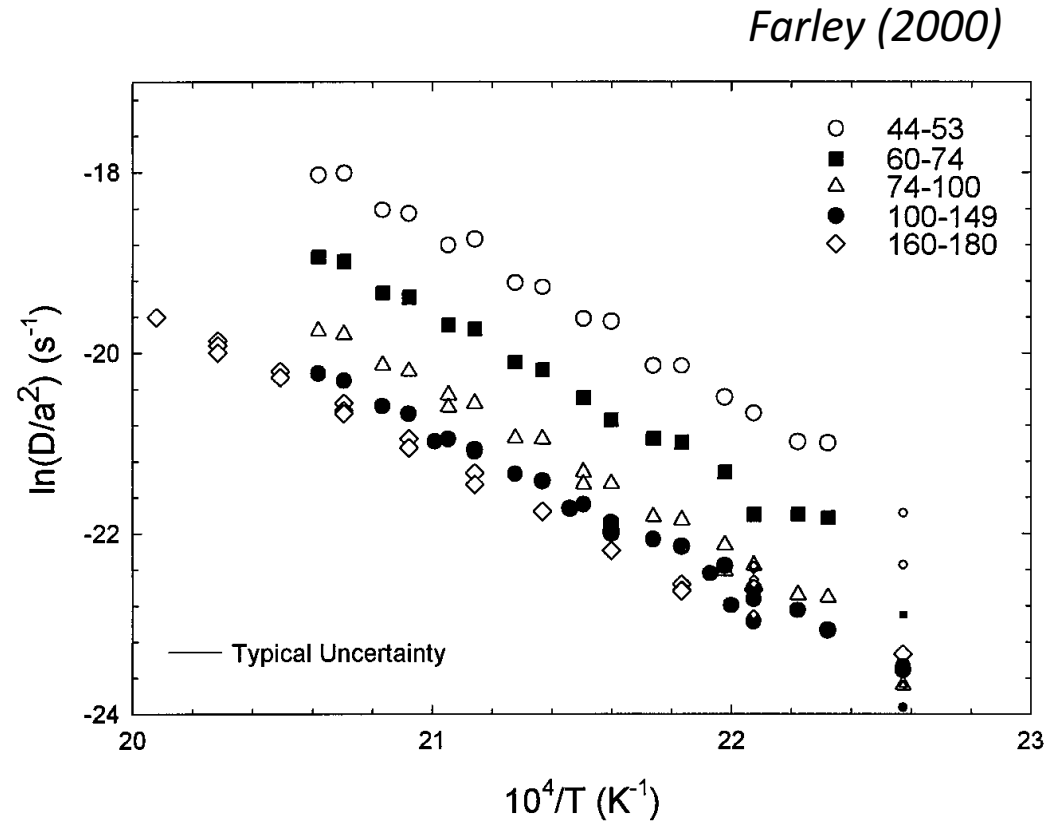


Reiners (2009)

II. Diffusion in a simple system : one crystal

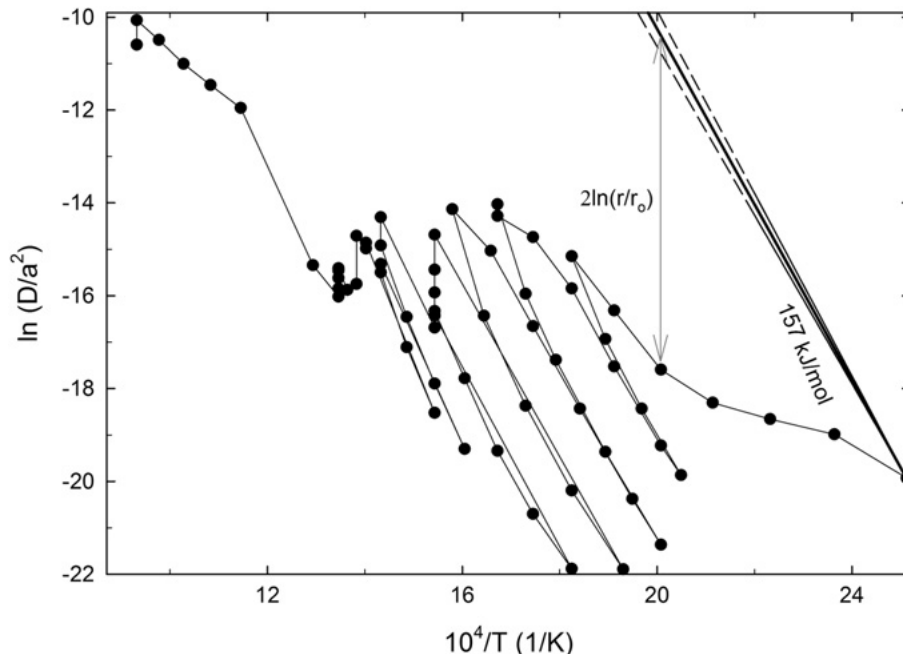
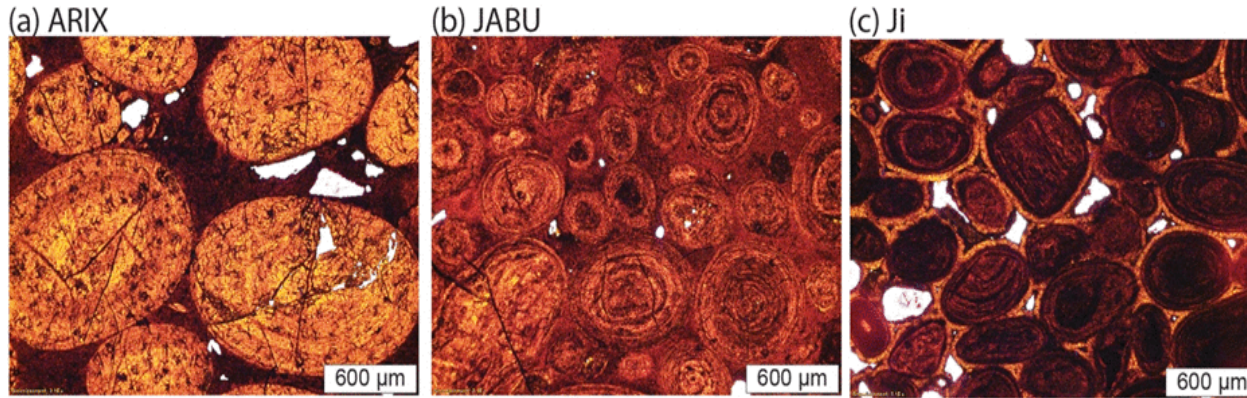


Ehlers and Farley (2003)



- The grain volume is the diffusion domain
- One crystal size (a)
- **Similar D_0 and E_a for all the grain size**

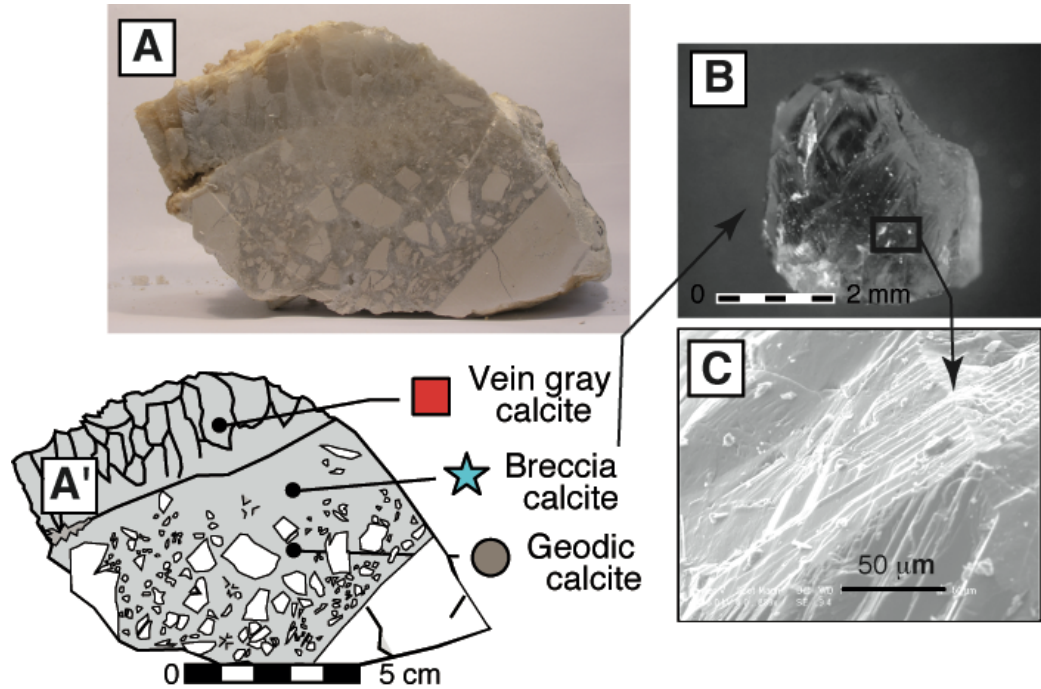
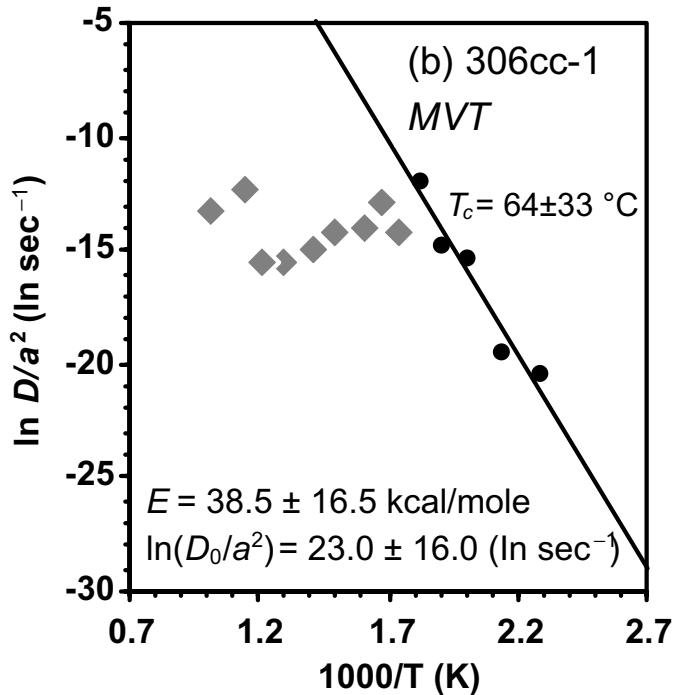
II. Diffusion in a complex system : polycrystalline structure



- Polycrystalline structure in iron oxide crystals (hematite and goethite)
- Different crystal sizes (a)
- Difficulty to determine D_0 and E_a

Farley and Flowers (2012)
Allard et al. (Submitted)

II. Diffusion in a complex system : fast paths

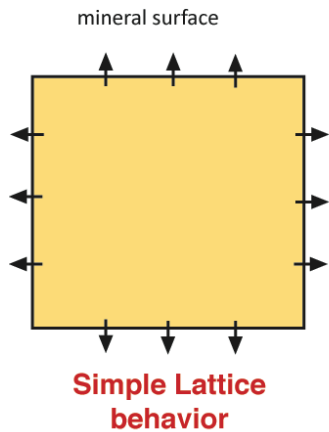
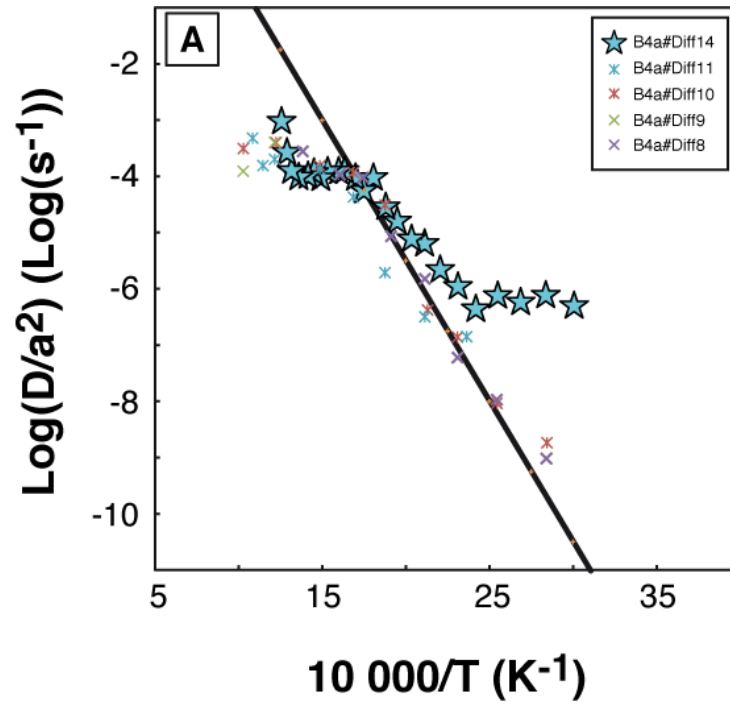


Breccia and fault filling calcite samples from the **Eocene/Oligocene Gondrecourt graben.**

Copeland et al. (2007);

Lovera et al. (1989, 1991); Cros et al. (2014)

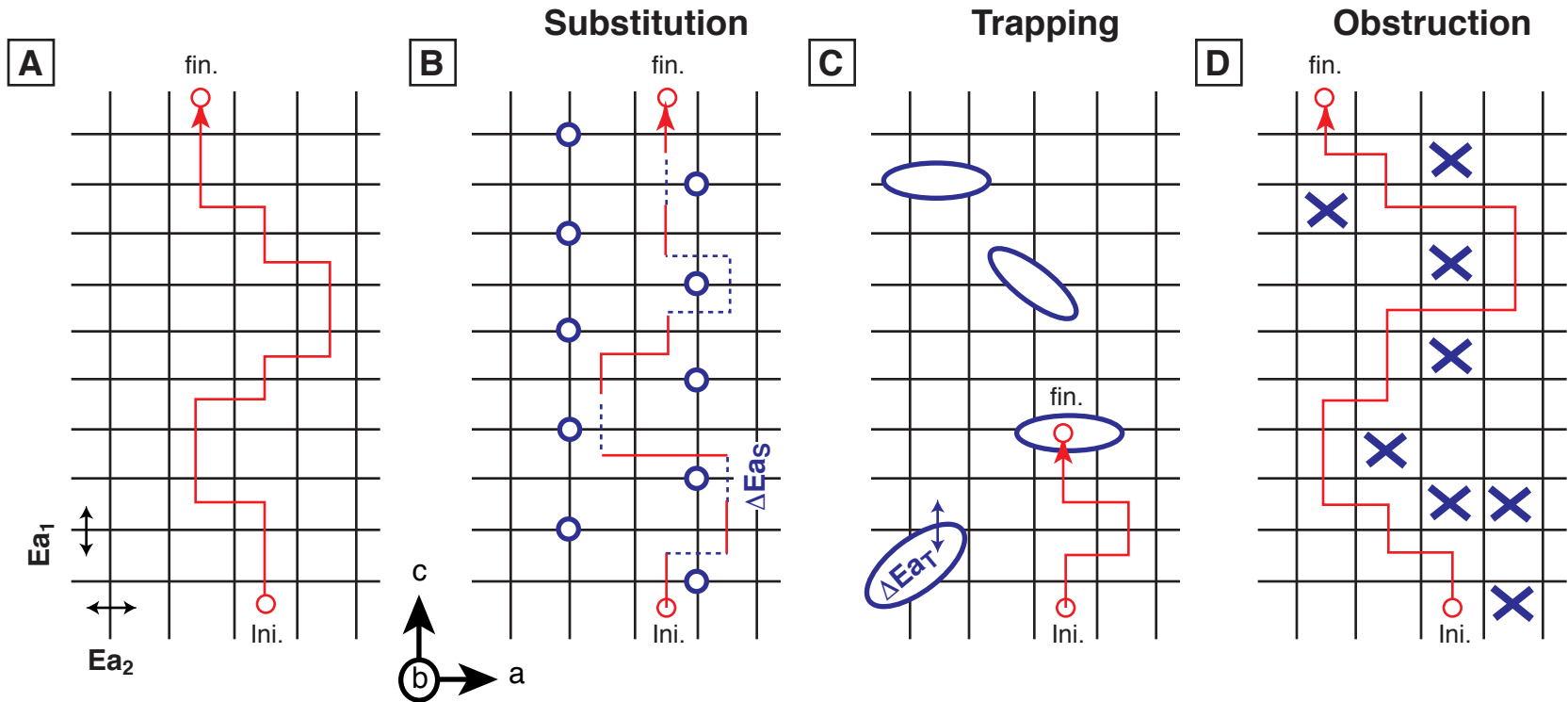
II. Diffusion in a complex system : use of a MDD model.



Lovera et al. (1989; 1991); Gautheron and Tassan-Got (2010); Cros et al. (2014)

II. Diffusion in a complex system: some hypotheses

- Different parameters can influence diffusivity in a crystal:



Gautheron et al. (in prep.)

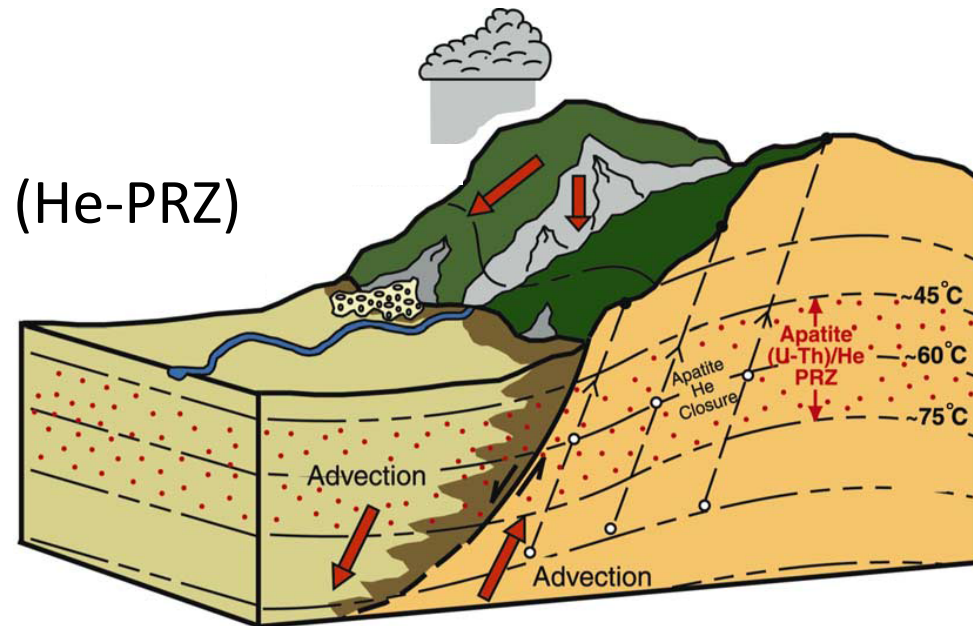
II. From diffusion coefficient to useable data

➤ He retention in crystal depends on:

1. Grain size (a)
2. Diffusion coefficient (D_0, E_a)
3. Thermal history ($T-t$)

➤ Need to get useable values such as of:

1. Closure temperature (T_c)
2. He Partial Retention Zone (He-PRZ)



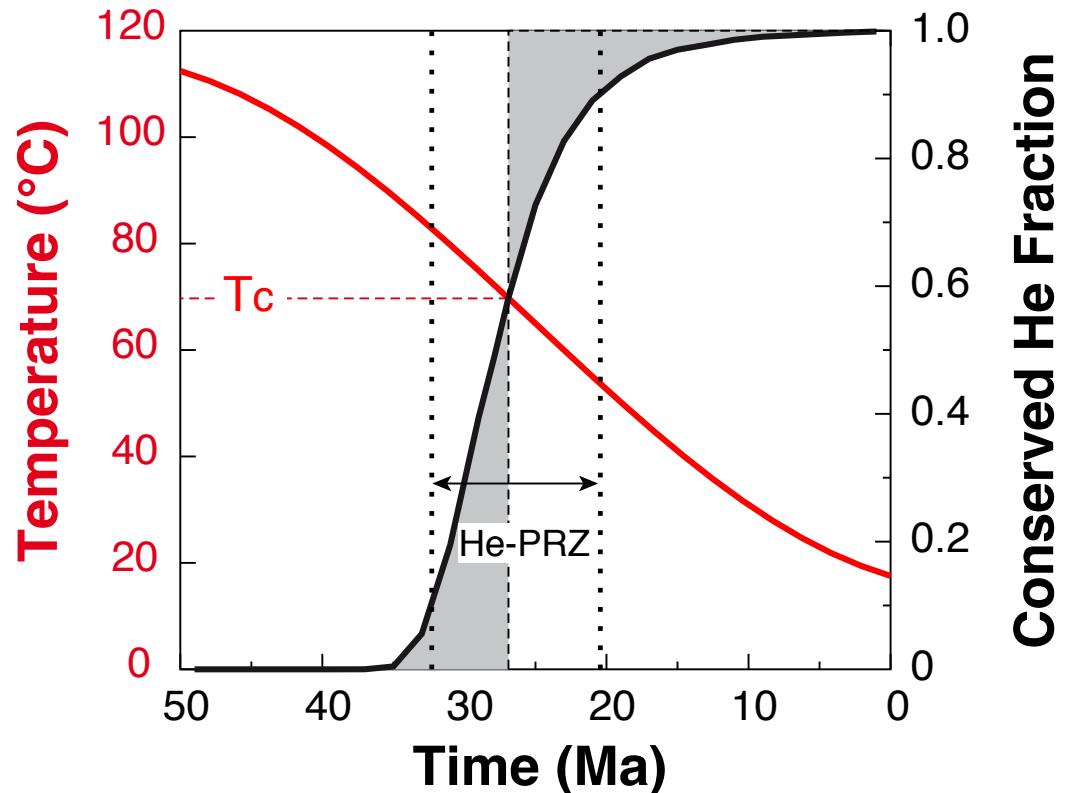
II. Closure temperature and He-PRZ

- **T_c**: when 50% of produced He atoms is retained in the crystal
- **He-PRZ**: between 10 to 90% of the retained He

$$T_c = \frac{E_a}{R \ln \left(A \tau \frac{D_0}{a^2} \right)}$$

$$\tau = \frac{RT_c^2}{E_a T}$$

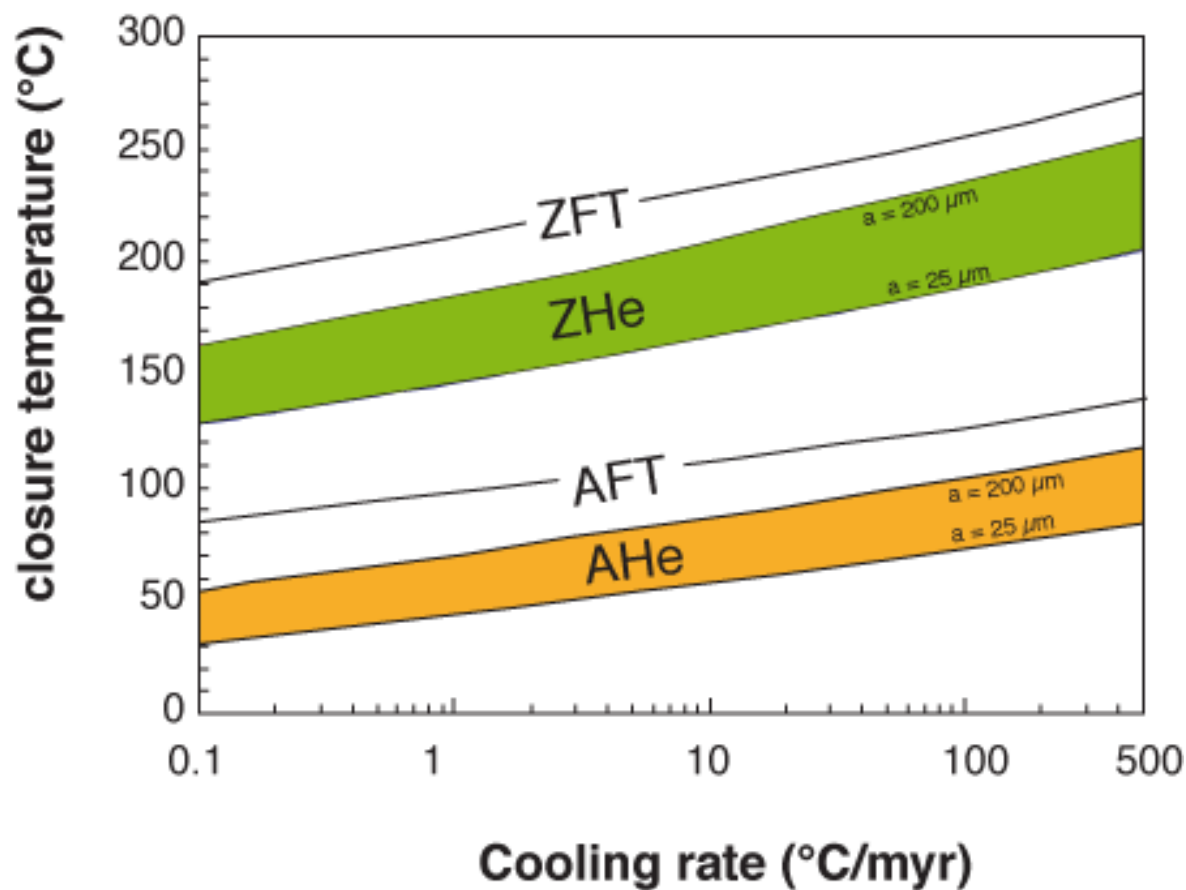
Dodson (1973)



➤ **See EXERCICE 1**

Using Gautheron and Tassan-Got (2010) code

II. Closure temperature example



Modified from Reiners (2005)

➤ $T_c = f(D_0, E_a, \text{cooling rate, grain size})$

II. Closure temperature and He-PRZ

TAKE HOME MESSAGE:

- (U-Th-Sm)/He age is not the time when rock crosses the closure temperature (T_c) or very rarely
- **Diffusion domain** and diffusion **coefficient** strongly influence thermochronometric age

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(2) How to get an (U-Th)/He age

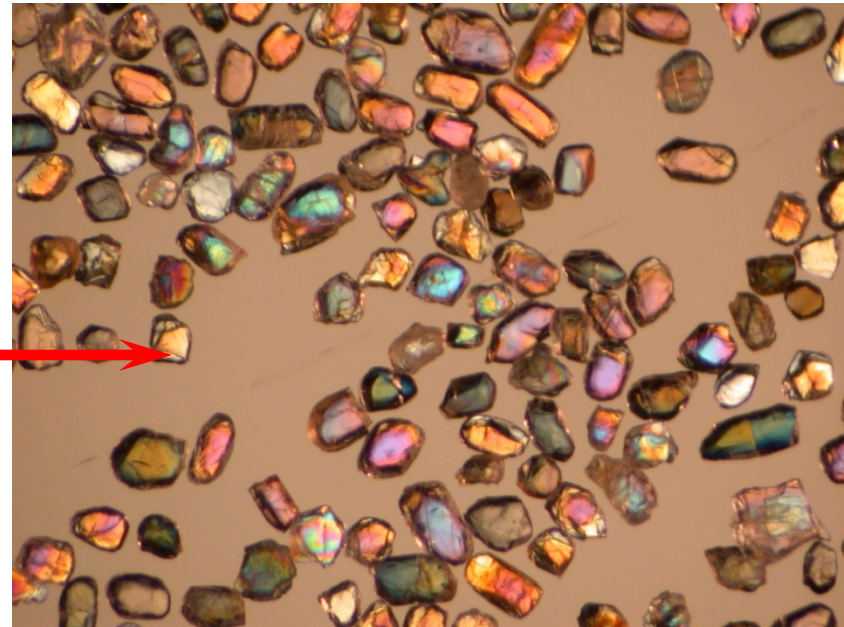
(3) Applications

III. Apatite (U-Th-Sm)/He (AHe) method

IV. Other applications (zircon, iron oxides,...)

(4) Exercises (Tc, ejection, weight, Rs), thermal modeling

(2) From sample to grain separation



Crushing, sieving, cleaning...

Need of 1 to 10 kg of rock to obtain enough “datable” apatite grains

(2) Grain selection



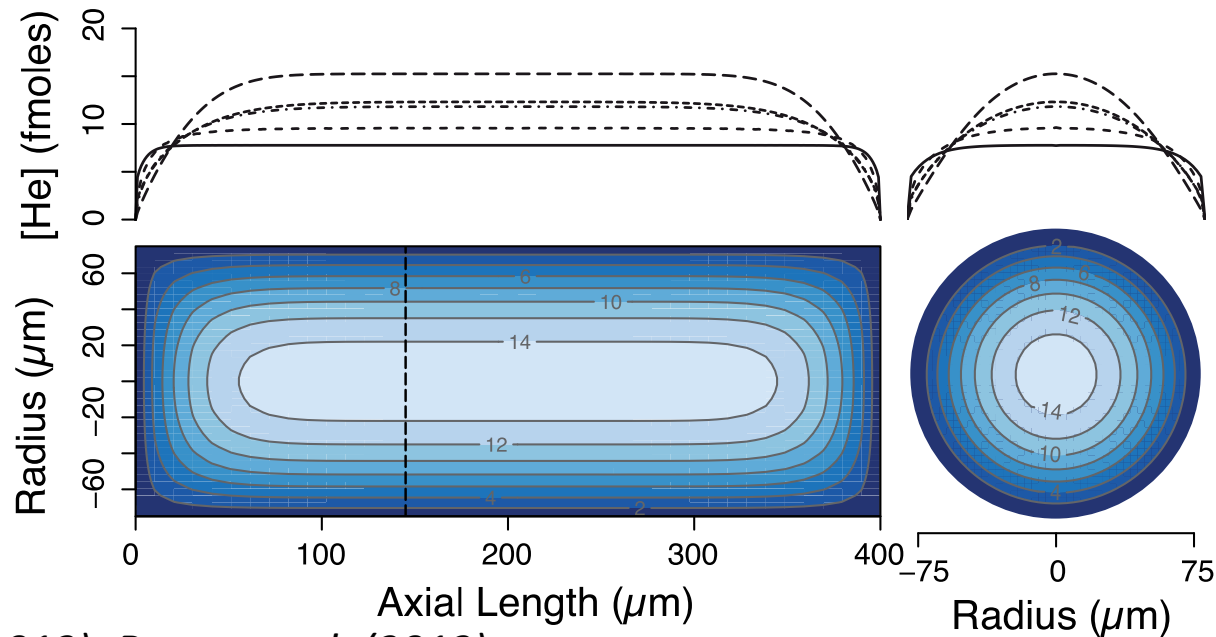
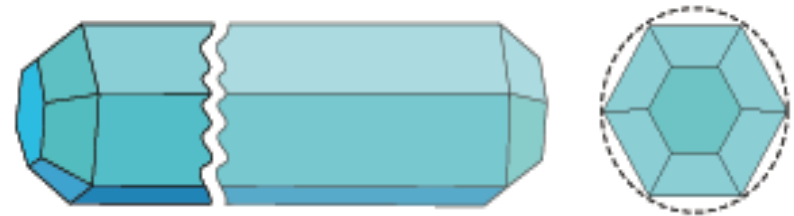
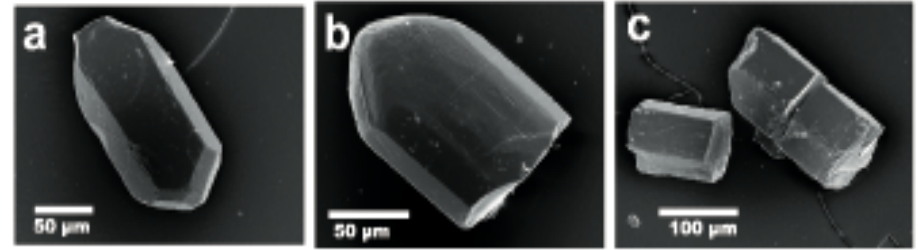
Ehlers and Farley (2003)

Drastic apatite selection criterion, grain size measurement + geometries (pyramids, broken faces)

(2) Grain morphology impact on AHe age interpretation

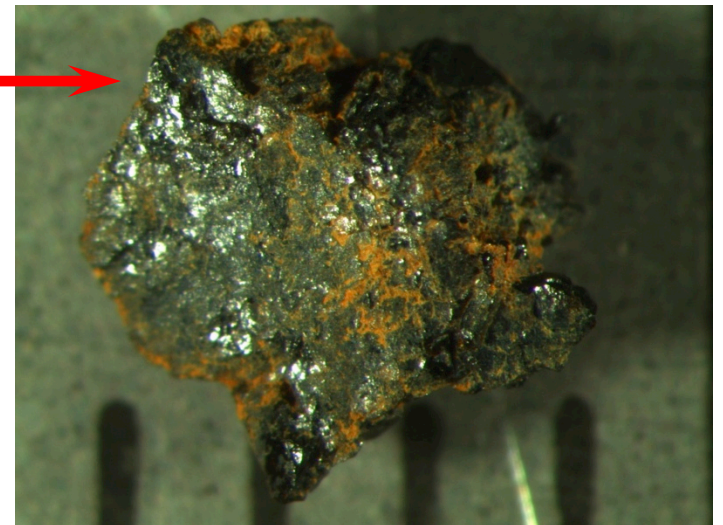
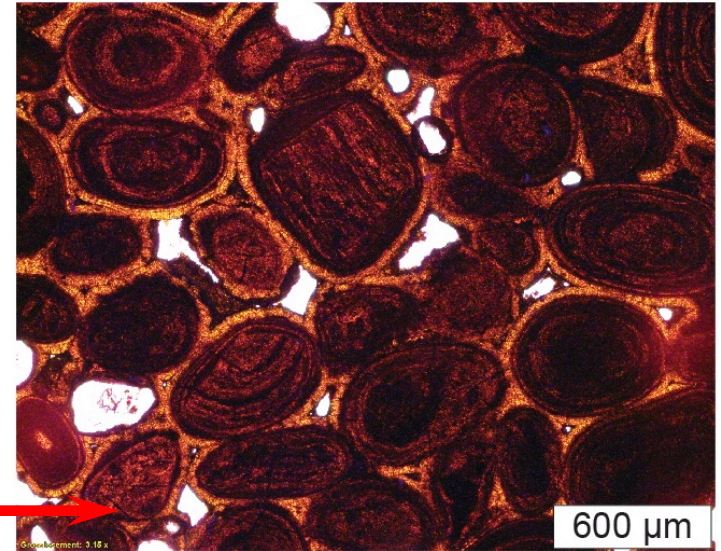
AHe age will be impacted by:

1. Crystal size (L, H, W),
2. Grain morphology,
3. Broken faces



Beucher et al. (2013); Brown et al. (2013)

(2) From sample to grain separation



Iron oxide duricrusts or pisoliths
(crystallographic characterization)

(2) Alpha ejection correction factor (F_T)

Farley et al. (1996)

Alpha ejection correction factor F_T :

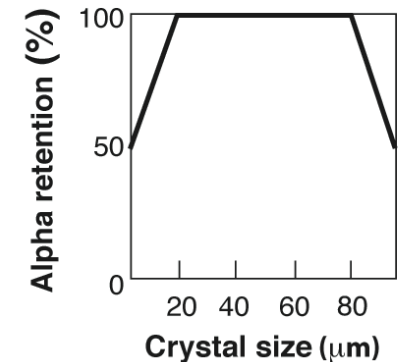
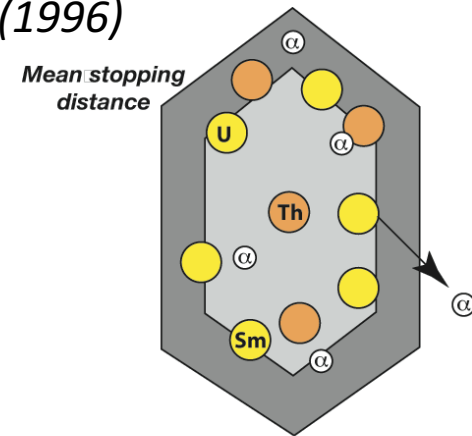
- sphere with homogeneous U-Th-Sm repartition

$$F_T = 1 - \frac{1}{4} \frac{SR}{V} = 1 - \frac{3}{4} \frac{R}{R_s}$$

For realistic geometries (2 approaches):

- Hexagonal \pm pyramids, for homogeneous U-Th-Sm

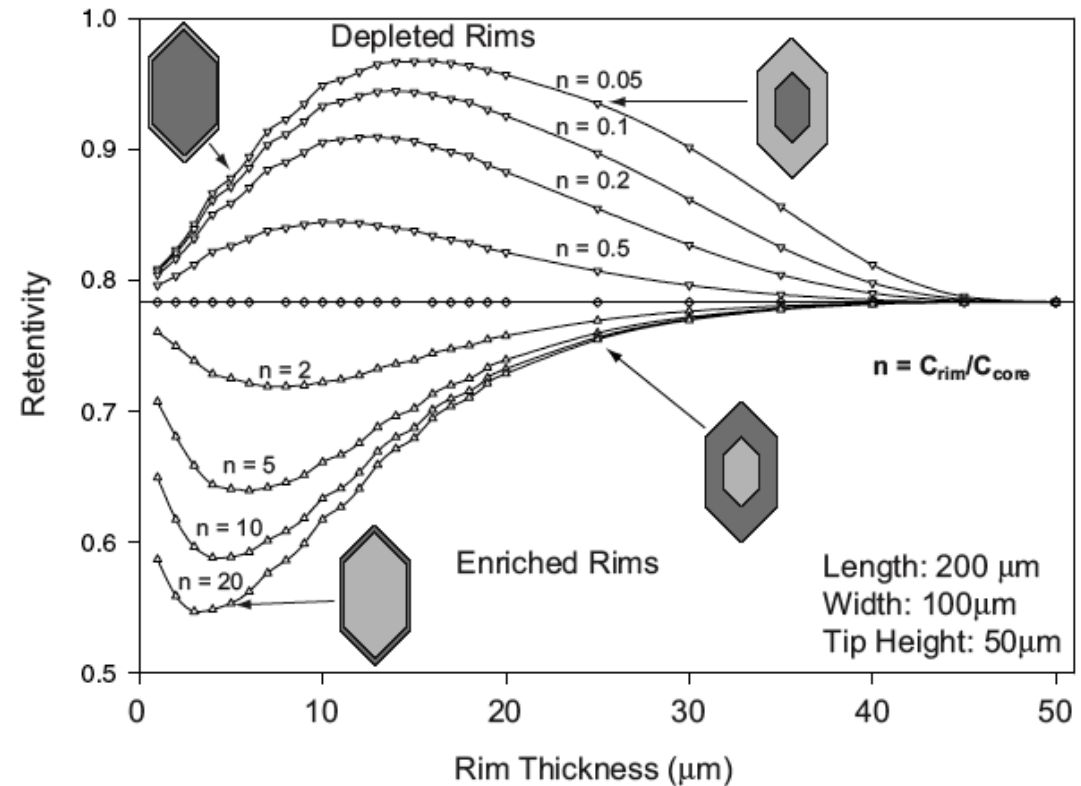
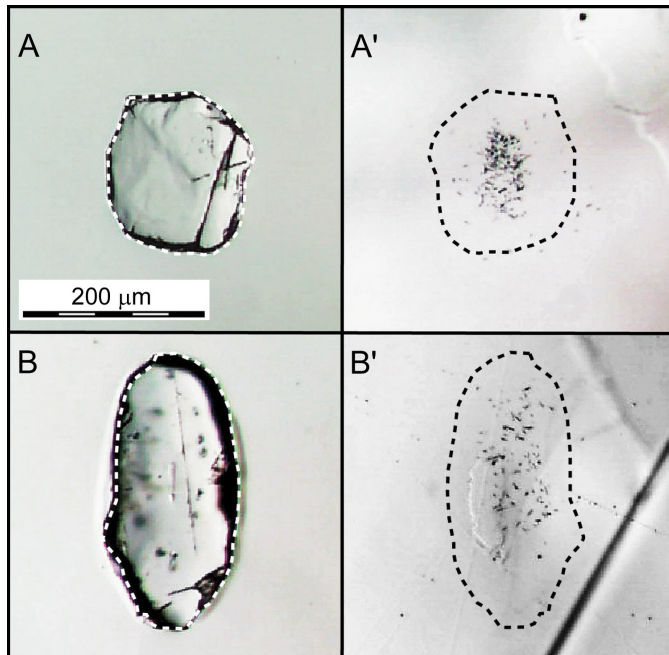
$$F_T = 1 - \frac{3}{4} \frac{R}{R_s} \left[\left(0.2093 - 0.0465 N_p \right) \left(W + \frac{L}{\sqrt{3}} \right) + \left(0.1062 + \frac{0.2334 R}{R + 6(W\sqrt{3} - L)} \right) \left(H - N_p \frac{W\sqrt{3/2} + L}{4} \right) \right] \frac{R^2}{V}$$



Ketcham et al. (2011)

(2) Alpha ejection correction factor: zoned U-Th-Sm crystals (F_{ZAC})

For crystals zoned in U-Th-Sm, F_{ZAC} factor can be determined analytically or using a Monte Carlo simulation



Vernon et al. (2009)

Hourigan et al. (2005)

(2) Correcting factor, weight, diffusion domain

Calculation using a Monte Carlo model of:

- Grain weight (μg)
- F_T , F_{ZAC} alpha ejection correction (0 to 1)
- R_s sphere equivalent radius (μm) for isotropic or anisotropic diffusion domain
 - Hexagonal (apatite)
 - Tetragonal (zircon)
 - \pm pyramids, broken faces
 - ...

Need of a $F_T > 0.65$ and $R_s > 40 \mu\text{m}$...

Alpha F_T -ejection factor
Cecile Gautheron, Laurent Tassan-Got and Richard Ketcham

Inputs

Geometry

Grain list

Grain	Shape
Grain 1	Regular Hexagonal
Grain 2	pyramid

Radius (μm) 100.0
H (μm) 300.0

New Grain
Delete Grain
Clear List

Zonation

use zonation Number : 1
N°: 1 ratio: 0.00 size: 0.0

Medium

apatite
 Default density
Density (g/cm³) 3.1

Alpha List

ThU
Th/U 1.0

MC

Number of events 1000000

Compute Help Quit

Results

He Range (μm)	20.33	Actual density (g/cm ³)	3.10
FT	0.845	Mass (μg)	16.11
R_sph (μm)	90.7		

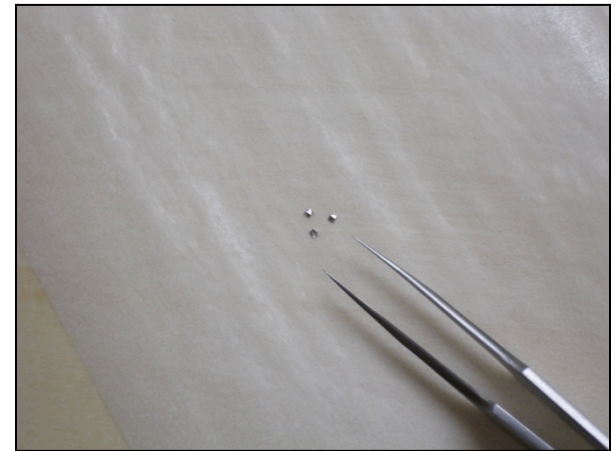
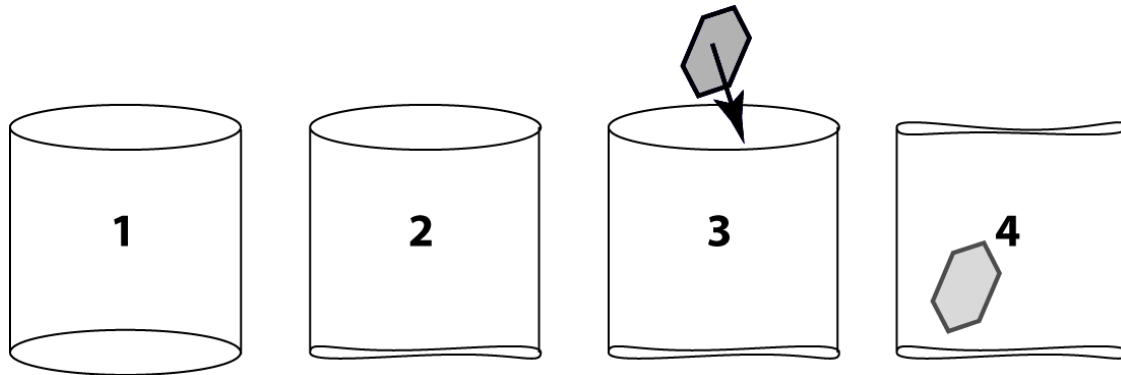
Ketcham et al., 2011, GCA, doi:10.1016/j.gca.2011.10.011
Gautheron and Tassan-Got, 2010, Chem. Geology, doi:10.1016/j.chemgeo.2010.02.023

Version date: 10/02/2012 based on Qt: <http://qt.nokia.com/>

Ketcham et al. (2011);
Gautheron et al. (2012)

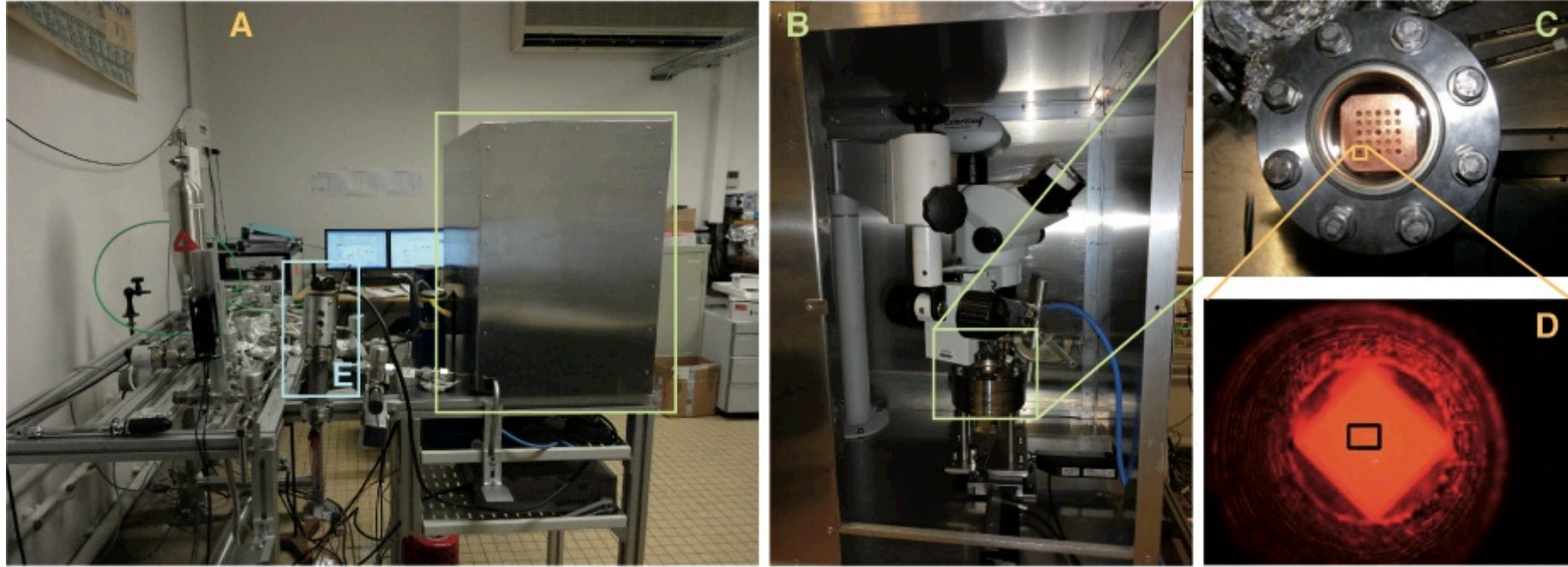
(2) Crystals packing: apatite , zircon, titanite... examples

Platinum tube (apatite), **niobium** tube (zircon, titanite) or **niobium** foil (iron oxides, calcite...)



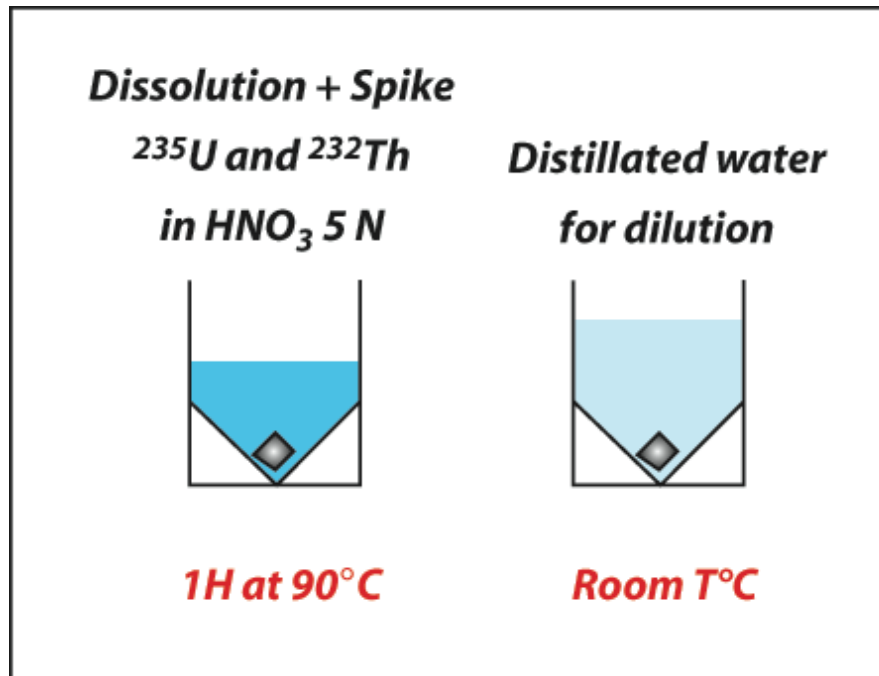
Capsule is used to transport the grain(s) and to ensure He degassing (laser light absorption).

(2) ^4He analysis



- Extraction, purification and analysis line for ^4He content determination at $\sim 2\%$
- Special gas purification for iron oxides (i.e. goethite) and calcite because of large H_2O and CO_2 degassing

(2) U-Th-Sm analysis



- Addition of pure selected isotopes (example: ^{235}U , ^{230}Th , ^{149}Sm) spikes during dissolution.

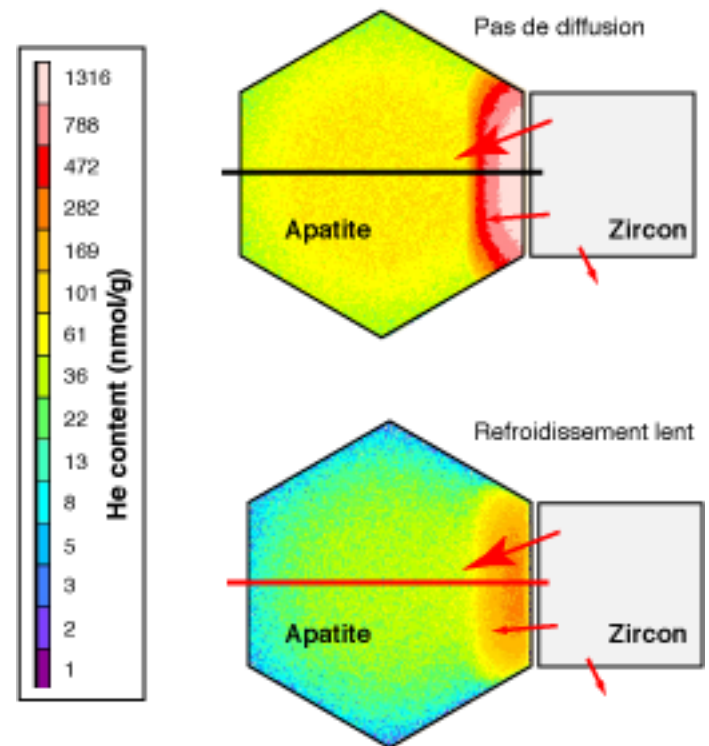
(2) U-Th-Sm analyses by ICPMS



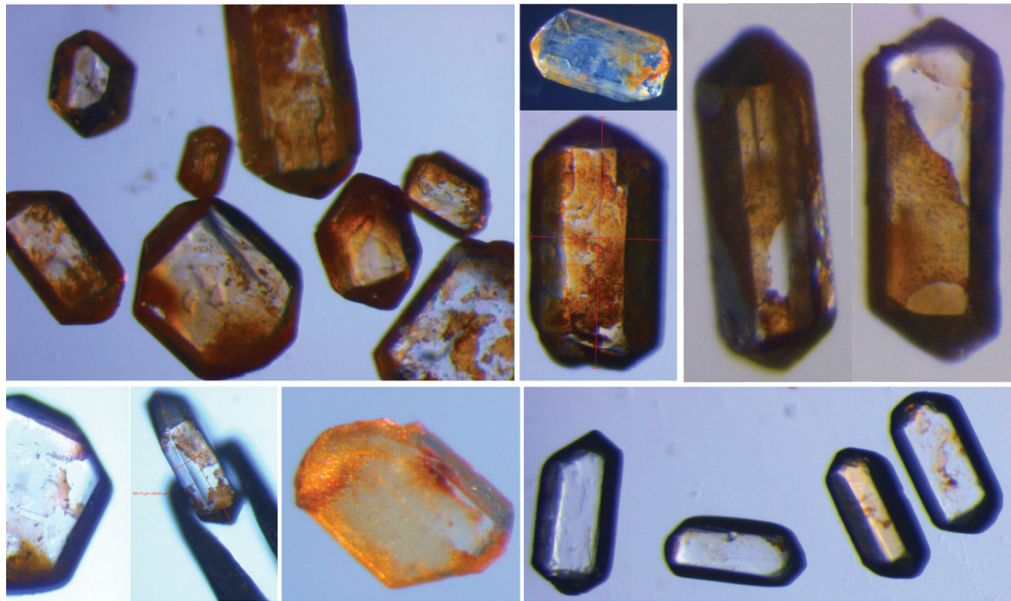
- ^{238}U , ^{232}Th and ^{147}Sm determination by isotopic dilution method (see Evans et al., 2005 for details)

(2) Base hypothesis

- U-Th decay series are on secular equilibrium ($t > 1\text{Ma}$)
- No U-Th-Sm loss
- No common helium, or ${}^4\text{He}$, ${}^{21}\text{Ne}_c \ll {}^4\text{He}^*$ (radiogenic)
- No ${}^4\text{He}$ implantation from neighbor minerals

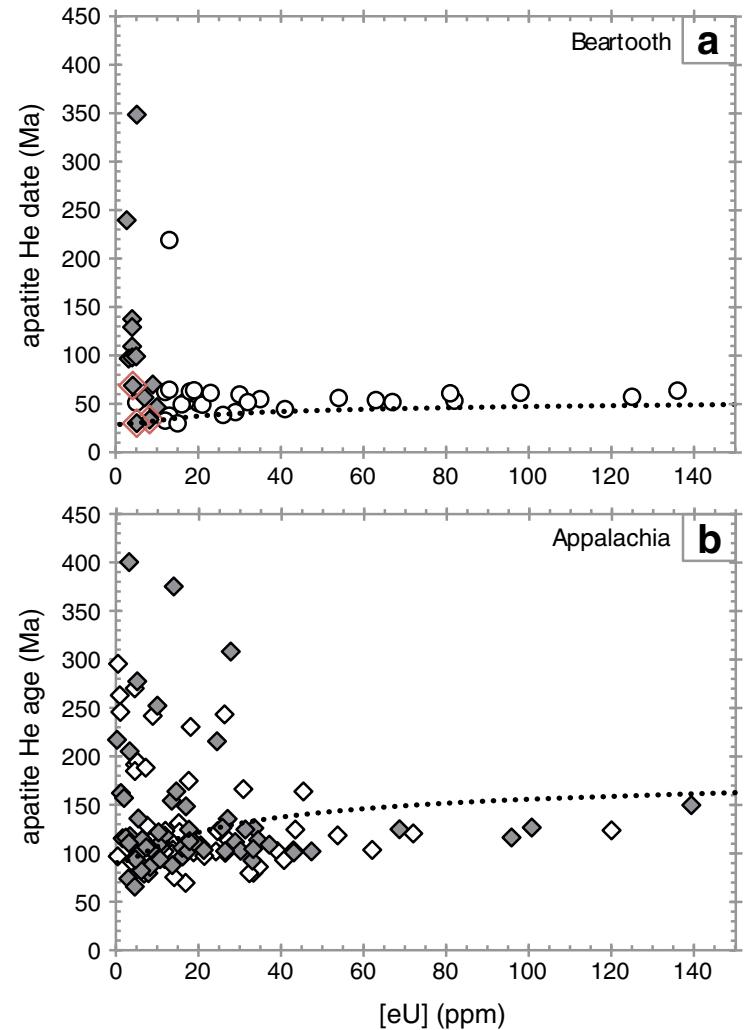


(2) Impact of He implantation on AHe age



From Murray et al. (2014);

See also Spiegel et al. (2009);
Janowski et al. (2017)



- reproducible or RDAAM-interpretable age trends
- ◇ highly-variable age trends
- ◇ GBP-coated grain
- RDAAM-predicted age-eU trends

(2) (U-Th-Sm)/He age calculation

1. (U-Th-Sm)/He age: $Raw\ age = \frac{[{}^4He]}{P^* (He\ production)}$

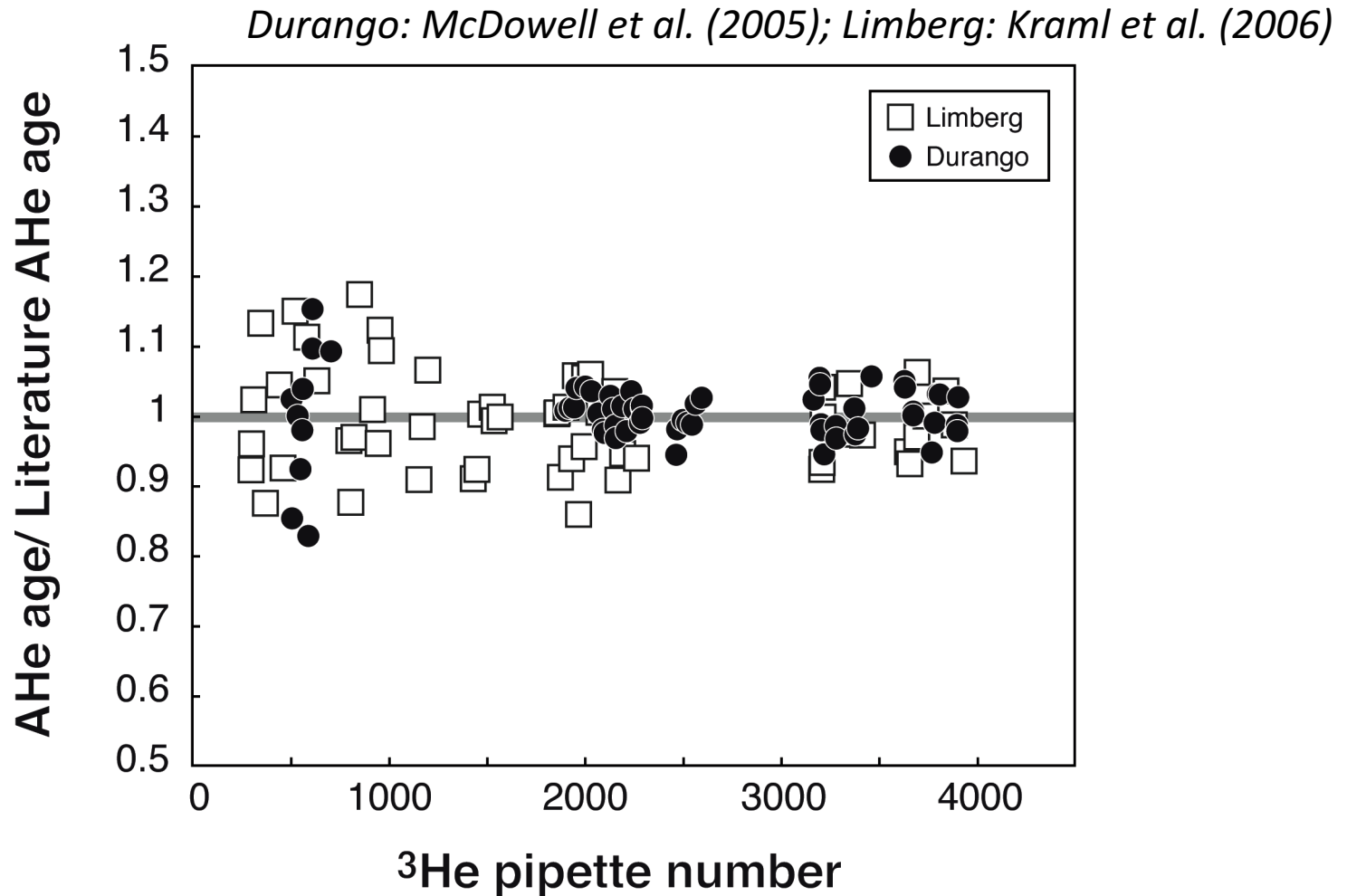
2. He instantaneous production (P^* / per year):

$$P^* = \left(8 \times \frac{137.88}{138.88} (e^{\lambda_{238} \times t} - 1) + 7 \times \frac{1}{138.88} (e^{\lambda_{235} \times t} - 1) \right) \times [U]$$
$$+ \left(6 \times (e^{\lambda_{232} \times t} - 1) \right) \times [Th] + \left(1 \times 0.1499 \times (e^{\lambda_{147} \times t} - 1) \right) \times [Sm]$$

3. Alpha ejection
corrected age:

$$Corrected\ age = \frac{Raw\ age}{F_T}$$

(2) He age reproducibility



- Analytical age: <4% = <2% for He and <2% for U-Th-Sm measurements
- Error on He age with ejection factor => 8-10%

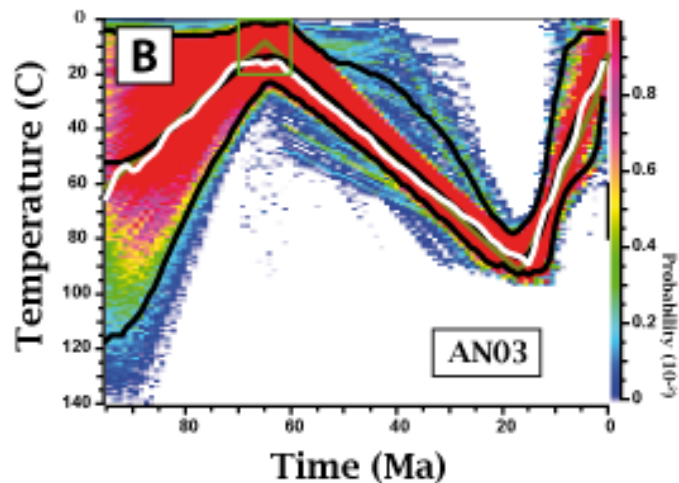
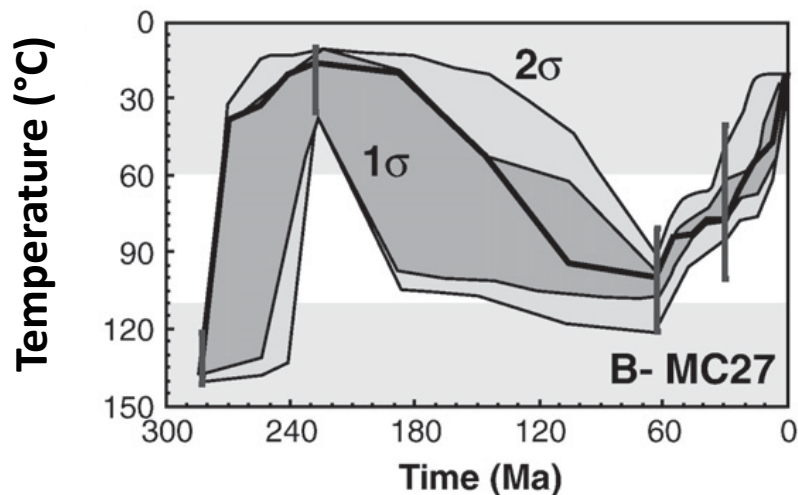
(2) Inversion of low temperature thermochronological data

→ **HeFTy** :

→ Tt path modeling

→ **QTQt** :

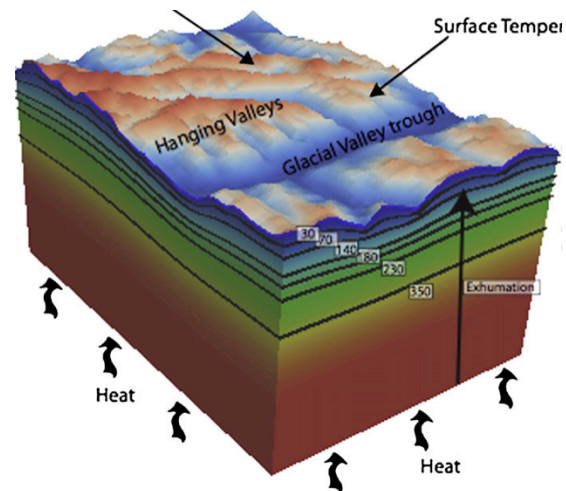
- Tt + pluri-samples (vertical profile) modeling



→ **PECUBE** :

- 3D modeling + vertical profile + faults ...

Ketcham (2005); Gallagher (2012); Braun (2003)



2) Data acquisition

TAKE HOME MESSAGE:

- **Do not underestimate** the time to **prepare and** pick your grains (especially for apatite)
- Measure all grains **geometry** and report all data (L, H, W, geometries)
- Error on (U-Th)/He age will be **~10%**

(1) (U-Th)/He dating system

I. Introduction, generalities

II. (U-Th)/He principles (chronometer vs thermochronometer)

(2) How to get an (U-Th)/He age

(3) Applications

III. Apatite (U-Th-Sm)/He (AHe) method

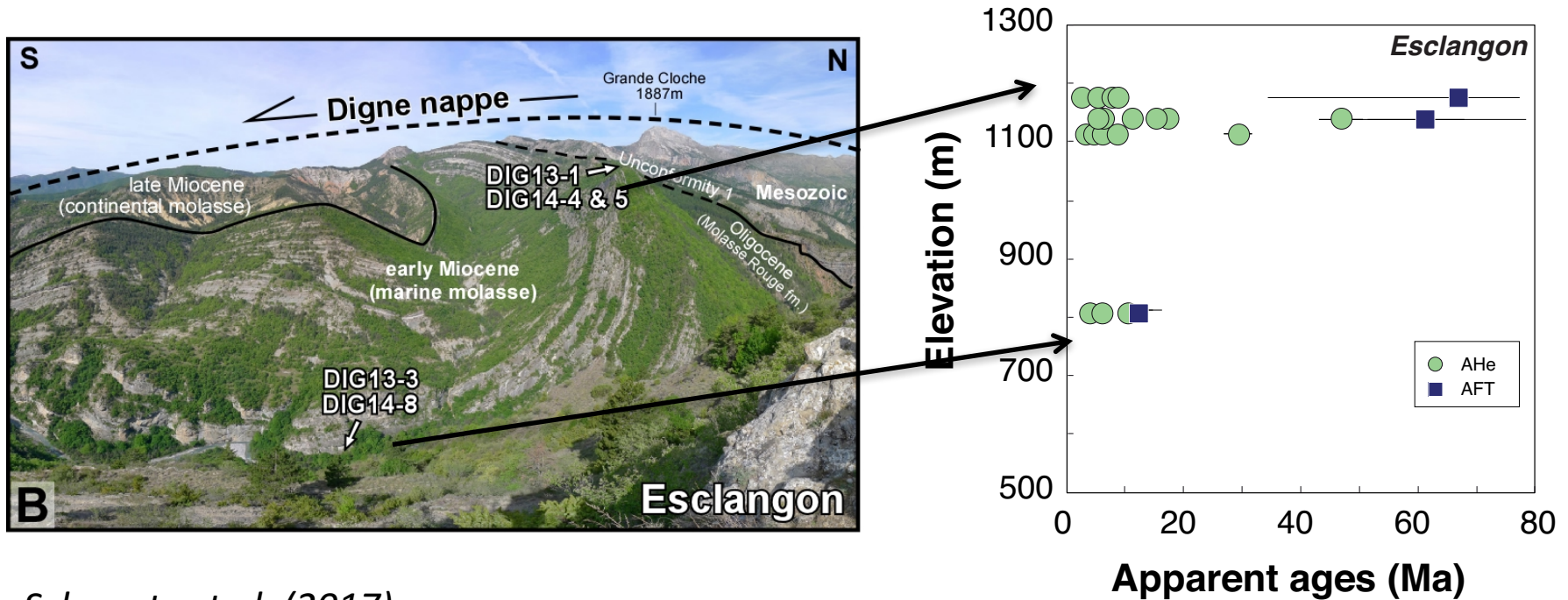
IV. Other applications (zircon, iron oxides,...)

(4) Exercises (Tc, ejection, weight, Rs), thermal modeling

III. Apatite He age distribution

➤ AHe age dispersion is often higher than analytical error (~8%)

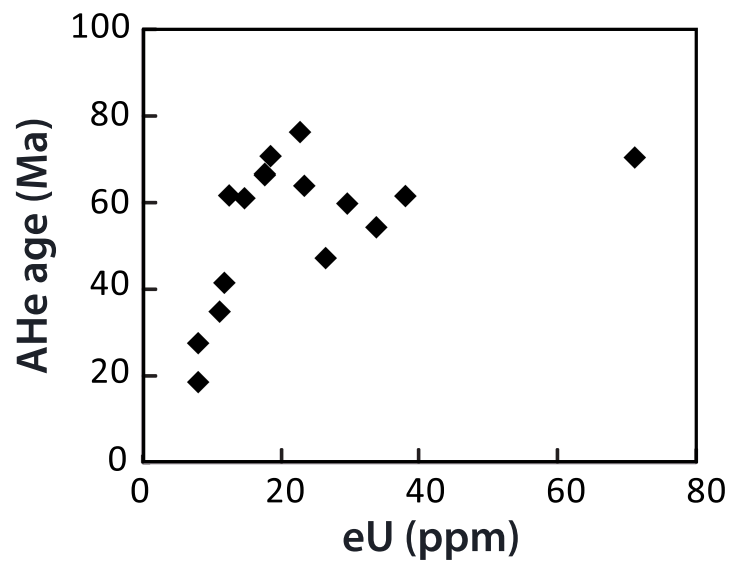
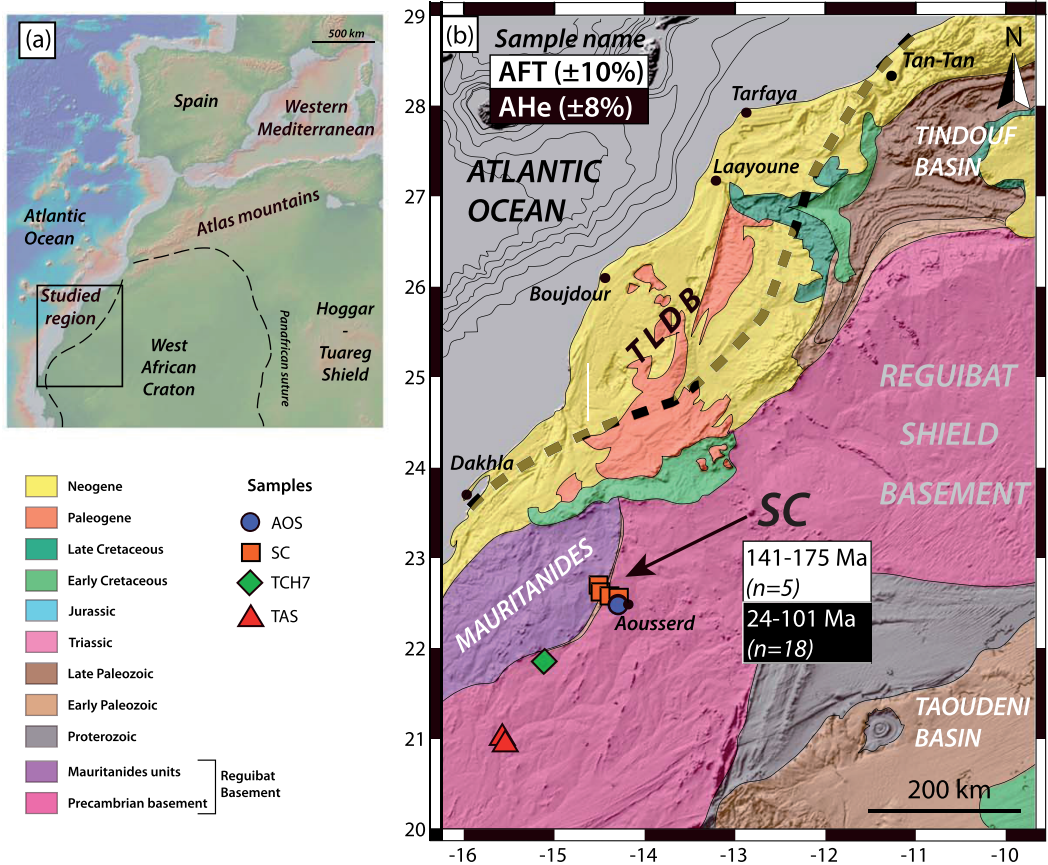
1. French foreland example (buried detrital apatite)



Important dispersion for higher elevation sample => **non total diffusion?**

III. Apatite He age distribution

2. Moroccan margin exhumed during Atlantic breakoff



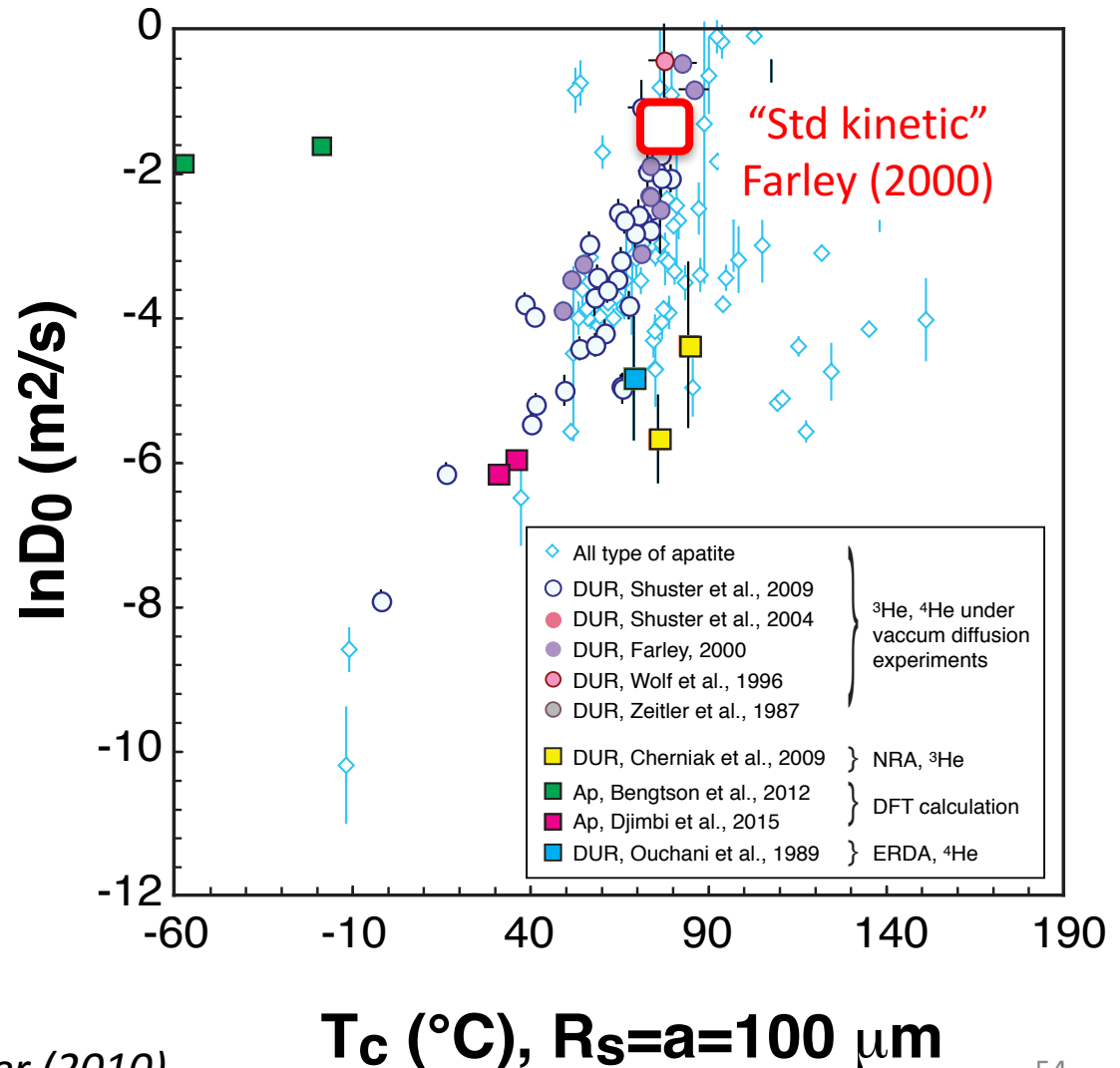
Leprêtre et al. (2015)

Important AHe age dispersion: relation with eU content?

III. Apatite He diffusion coefficient

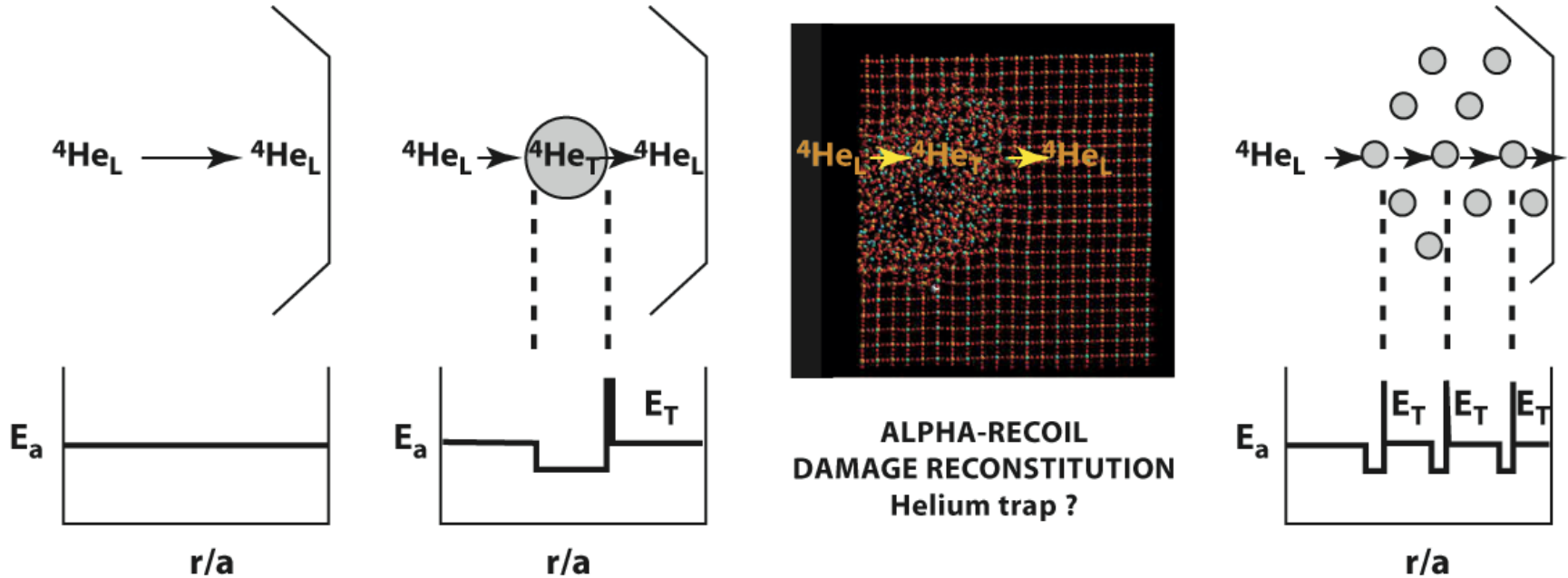
➤ Published He diffusion coefficient using different methods:

1. Under vacuum degassing experiments
2. Ion beam experiments
3. DFT calculation



Compiled 1987-2010 data by Baxter (2010)

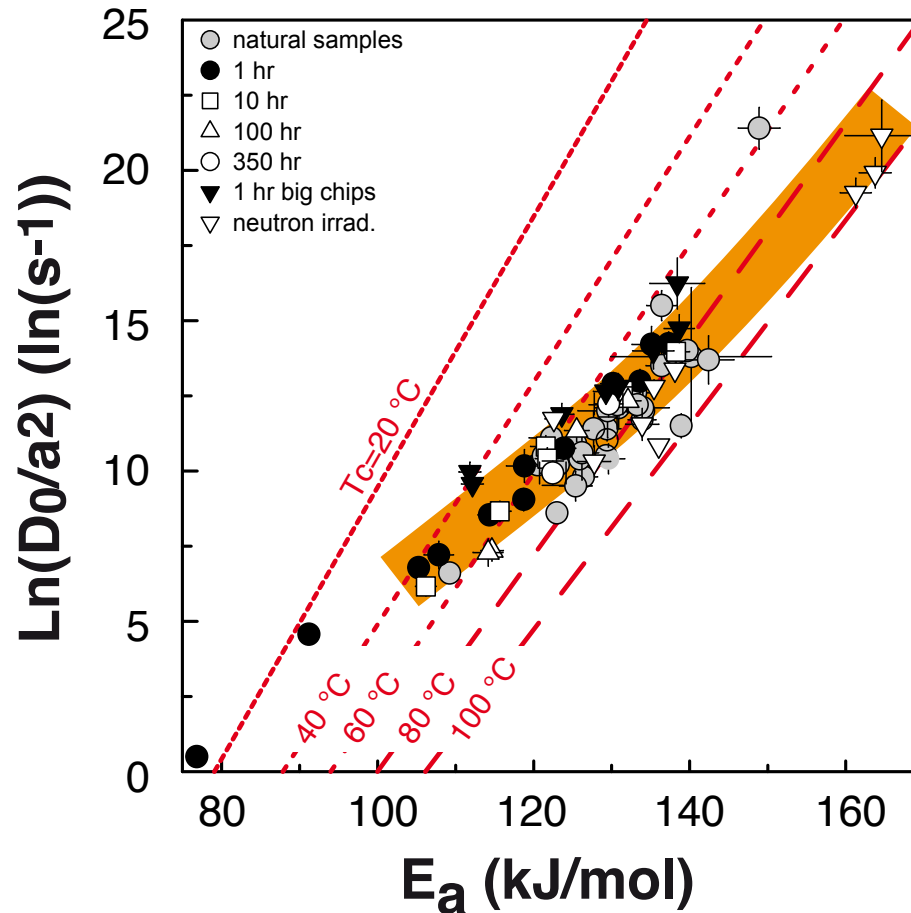
III. Relationship between eU and AHe age



*Shuster et al. (2006); Trachenko (2003);
See Green et al. (2006) for similar observation*

- Model where He atoms are trapped into damage zone => increase of He retention in apatite crystal and Tc value

III. Relationship between damage and diffusion coefficient

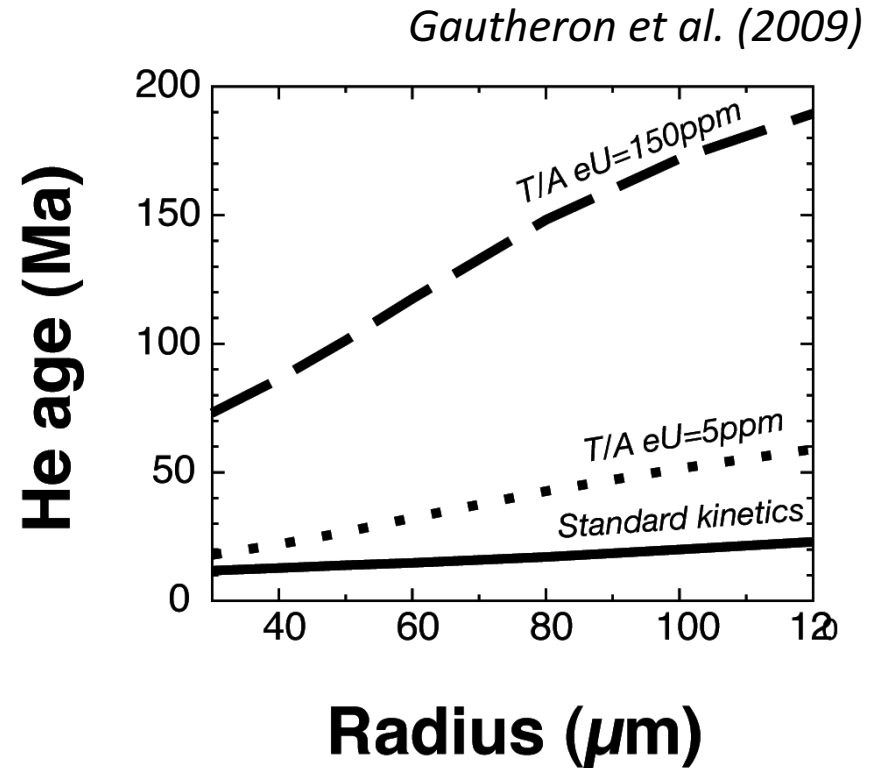
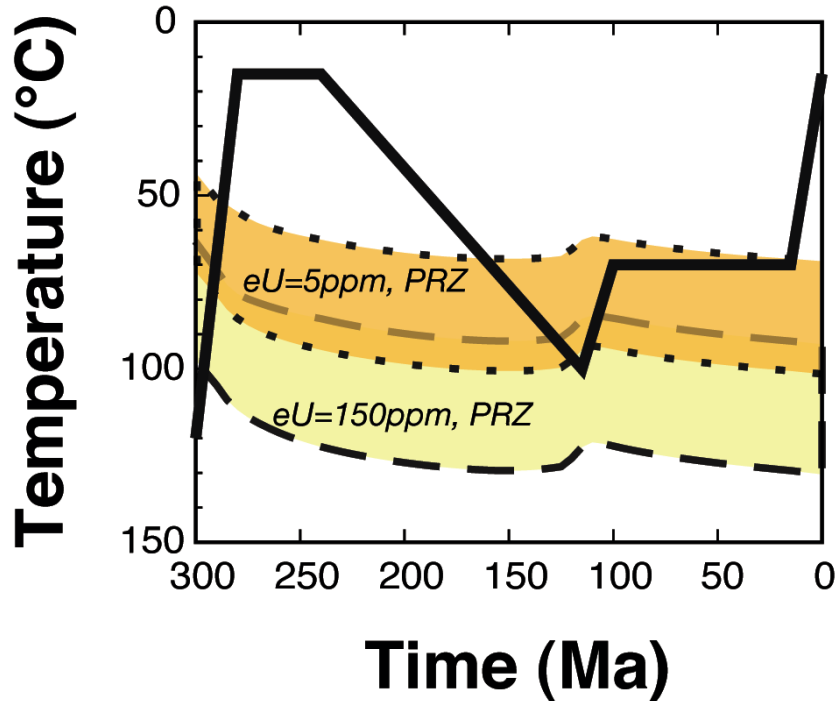


*Shuster et al. (2006);
Shuster and Farley (2009)*

- Empirical data showing the change of diffusion coefficient with artificial damage content

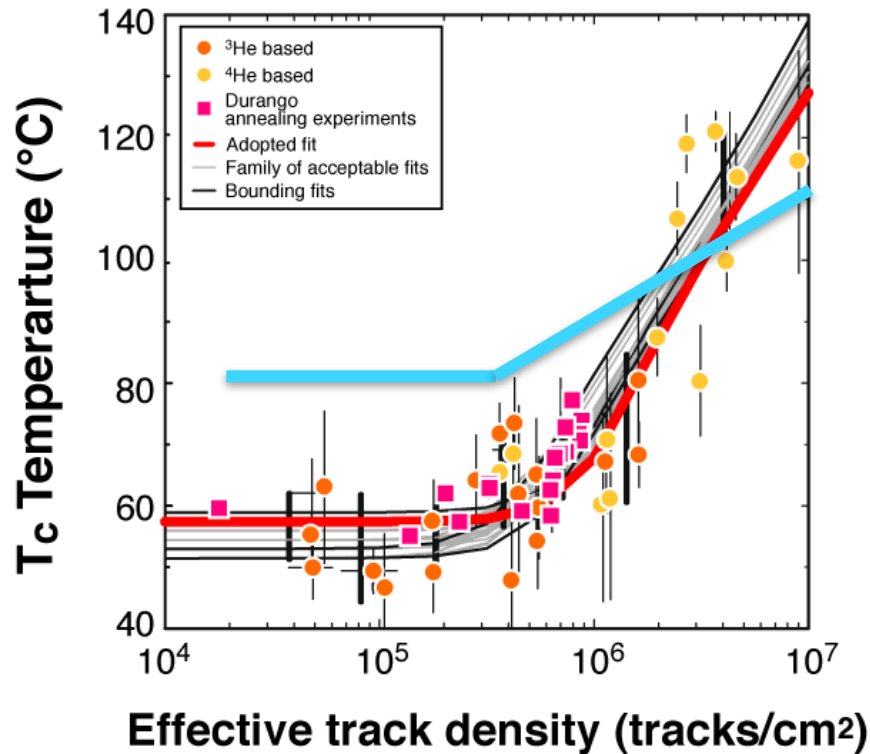
=> T_c ranges from 40 to > 100°C

III. Implication of damage content on He-PRZ



- Damage production and change of He diffusion, will change the Tc and He-PRZ through time

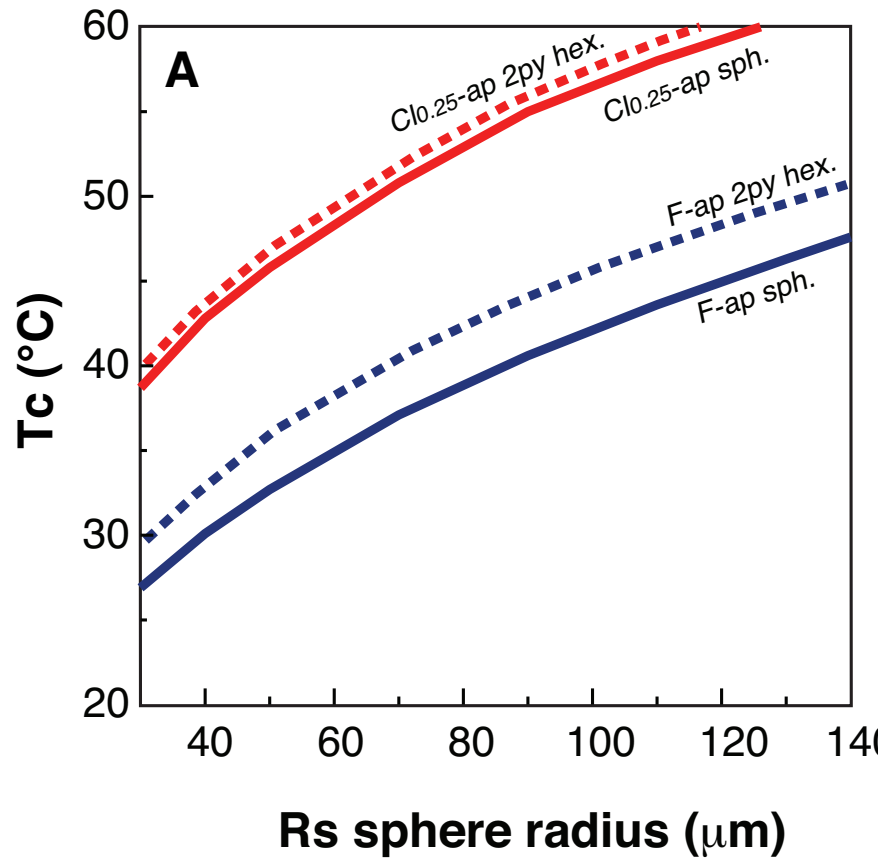
III. Diffusion in complex system: damage trapping + annealing model



Two damage + annealing models are used :

- Flowers et al. (2009): calibrated on natural + irradiated samples
- Gautheron et al. (2009): calibrated on “old” natural AHe ages

III. Chemical impact on diffusion

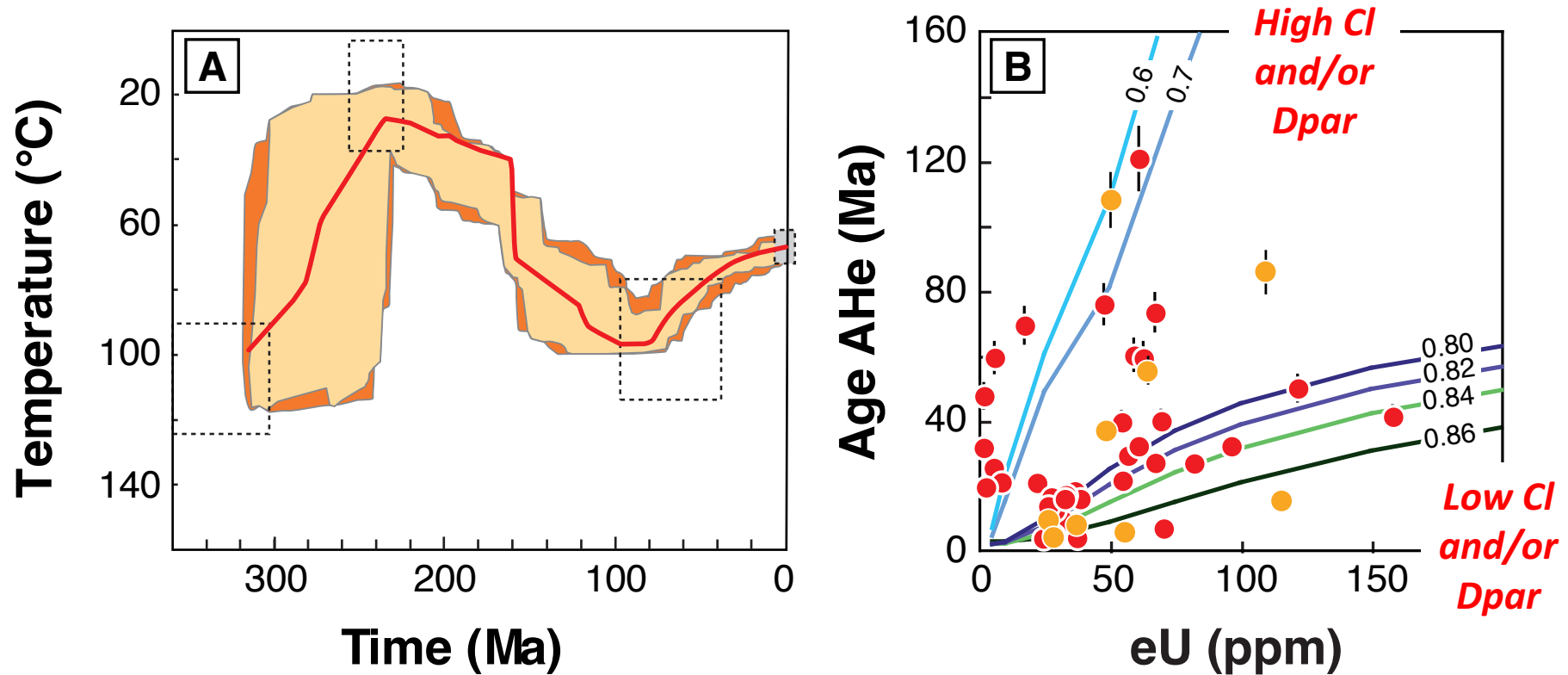


Djimbi et al. (2015)

- Chemical impact on He diffusion
- Lower Tc for undamaged apatite Tc=30-40°C

III. Chemical impact on diffusion

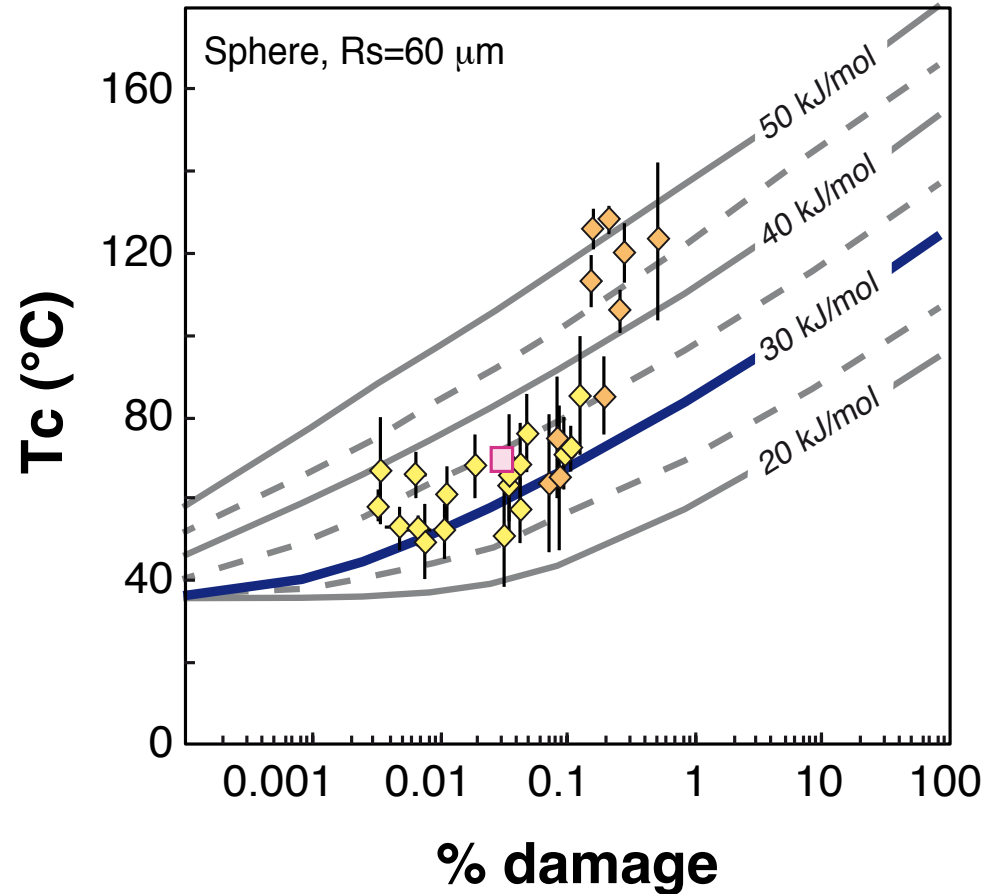
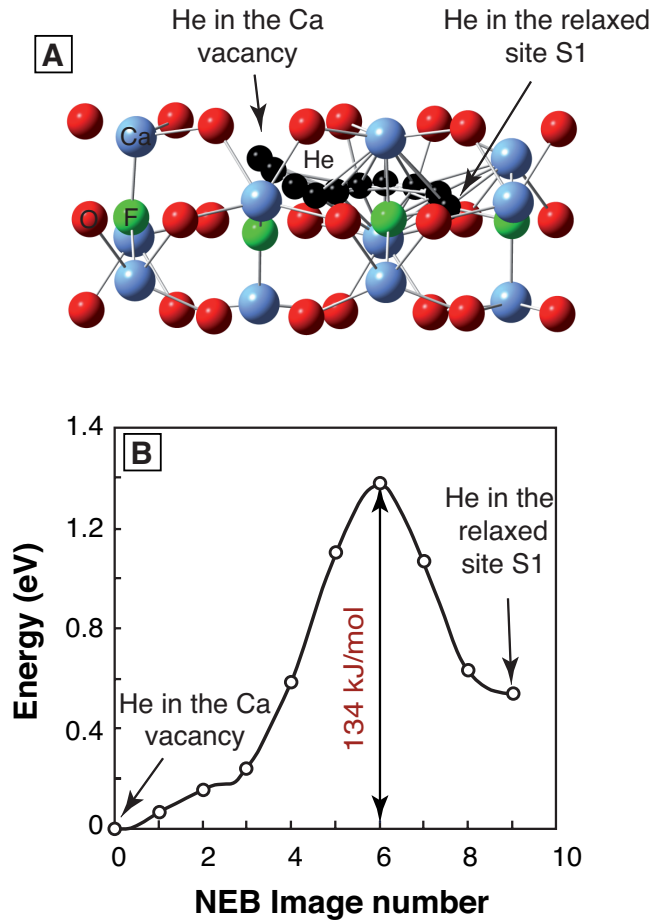
- Apatite chemistry play a role on damage annealing rate (such as for apatite fission tracks)



Modified from Gautheron et al. (2013);
Modeling: HeFTy Ketcham (2005) + Flowers et al. (2009)

(See EXERCICE 3)

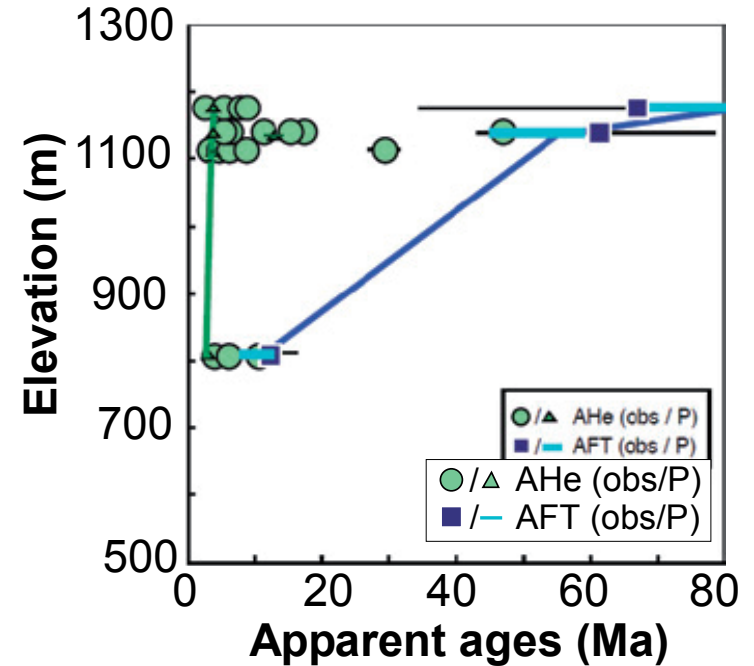
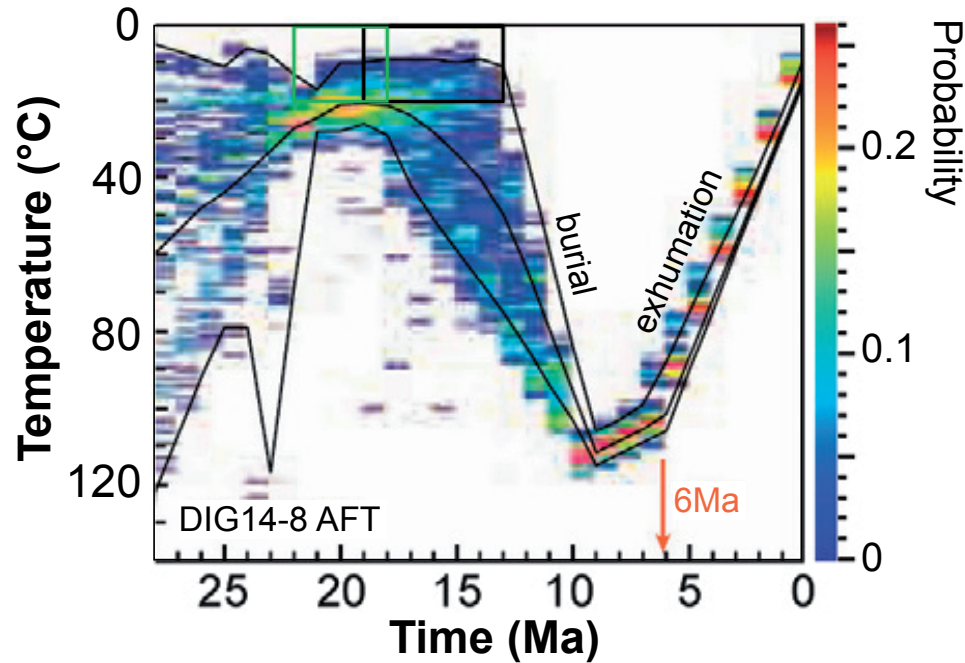
III. Damage impact on diffusion



Gerin et al. (2017)

- We are currently calibrating the new He damage model
- New code will be implemented into QTQt and HeFTy in 2018

III. Use of apatite He age dispersion

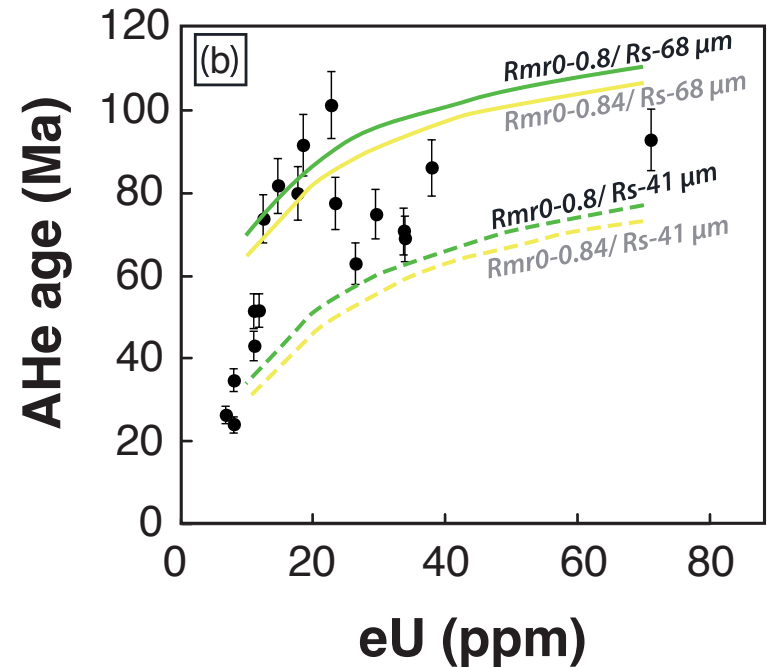
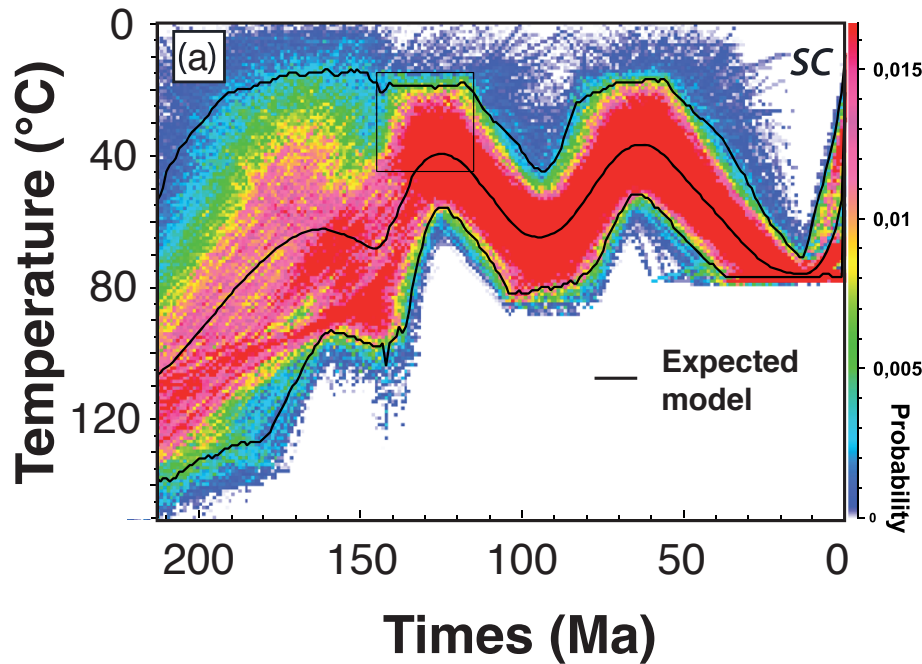


Schwartz et al. (2017)

Simulation QTQt (Gallagher, 2012), with Flowers et al. (2009) code

- AHe age dispersion is useful to refine not only the burial time and temperature

III. Impact of chemistry and grain size on AHe age dispersion



*Leprêtre et al. (2015);
QTQt simulation using AHe and AFT data (Gallagher (2012))*

- Need to consider grain chemistry variation in addition to grain size and damage model

III. AHe age interpretation

TAKE HOME MESSAGE:

- **A geological meaning is associated with AHe age dispersion** as the age reflects the impact of:
 1. Grain size (diffusion domain)
 2. Damage content (eU + time + annealing via chemistry)
 3. Thermal history

- **Adapt the number of analyzed grains** as a function of thermal history (3 to > 10 apatite crystals)

(1) (U-Th)/He dating system

I. Introduction, generalities

II. (U-Th)/He principles (chronometer vs thermochronometer)

(2) How to get an (U-Th)/He age

(3) Applications

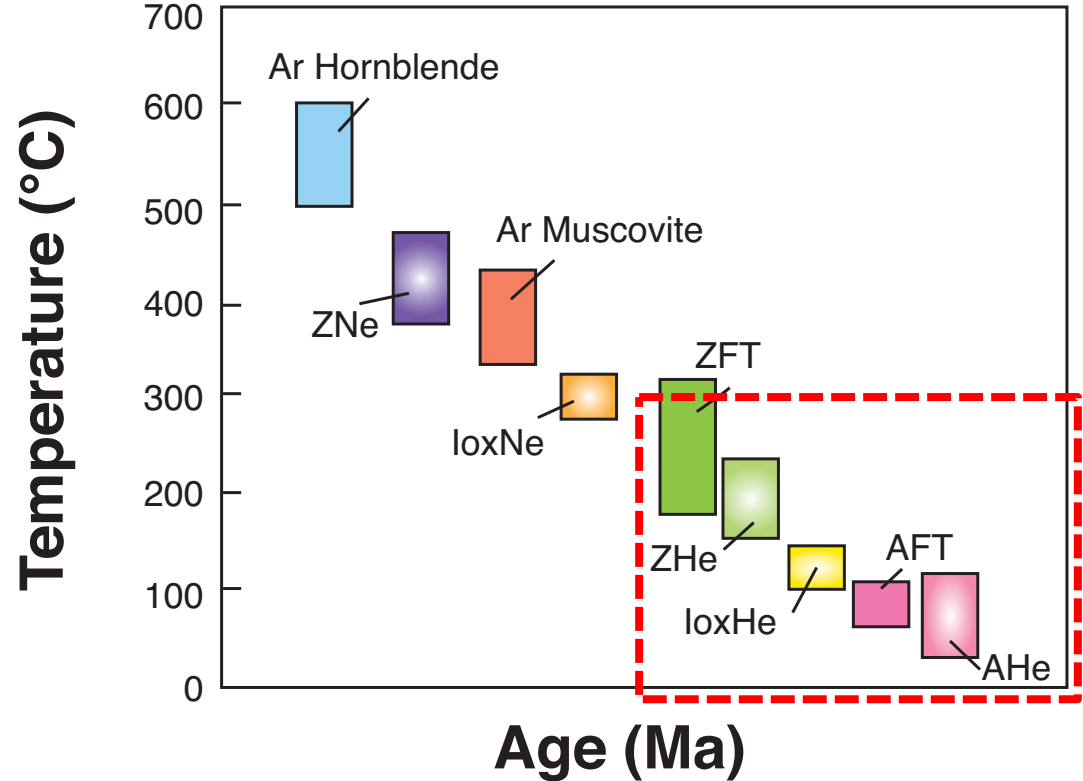
III. Apatite (U-Th-Sm)/He (AHe) method

IV. Other applications (zircon, iron oxides,...)

(4) Exercises (Tc, ejection, weight, Rs), thermal modeling

IV. Others applications

- (U-Th)/He system can be applied to a large range of minerals



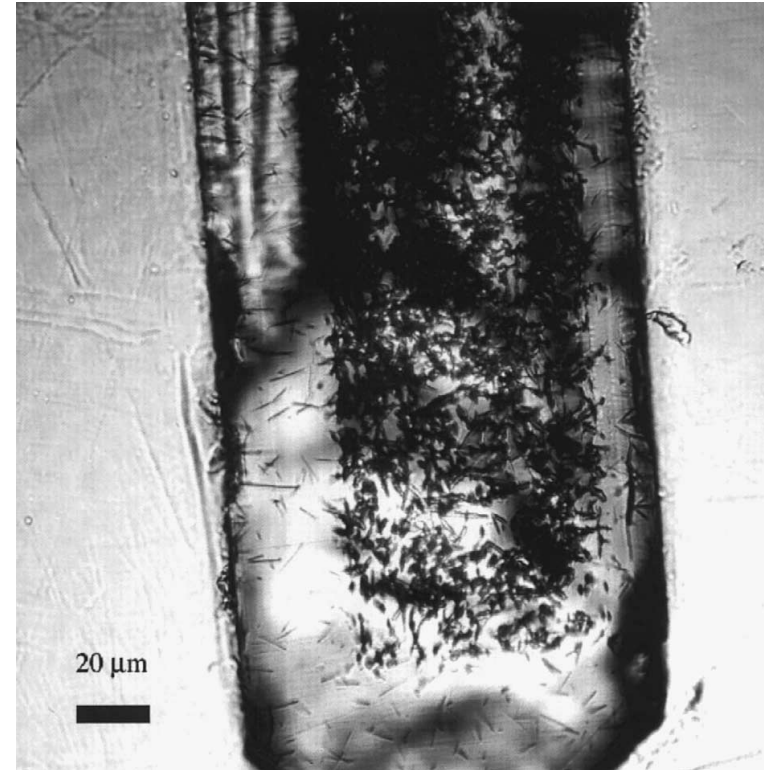
Which geological application ?

1. Higher temperature information than apatite => zircon, titanite
2. Ore deposit, laterite dating => goethite, hematite, magnetite

IV. Zircon (U-Th)/He (ZHe) method

➤ Zircon crystal can be found in a large variety of rocks (plutonic, volcanic and sedimentary)

1. Rich U-Th content: eU= 100 to 3000 ppm (He production from Sm is “null”)
2. U-Th zoned crystal
3. Lower stopping distance

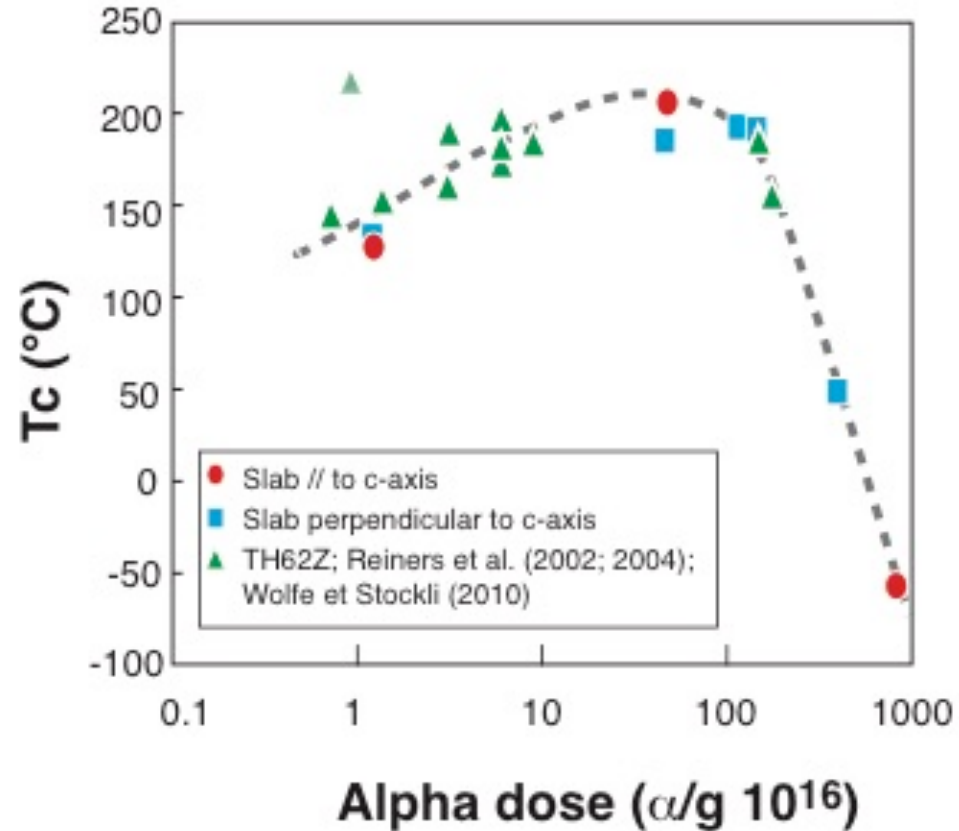


Tagami et al. (2003)

IV. Zircon (U-Th)/He (ZHe) method

➤ $T_c = 140\text{-}200^\circ\text{C}$ ($>AHe$)

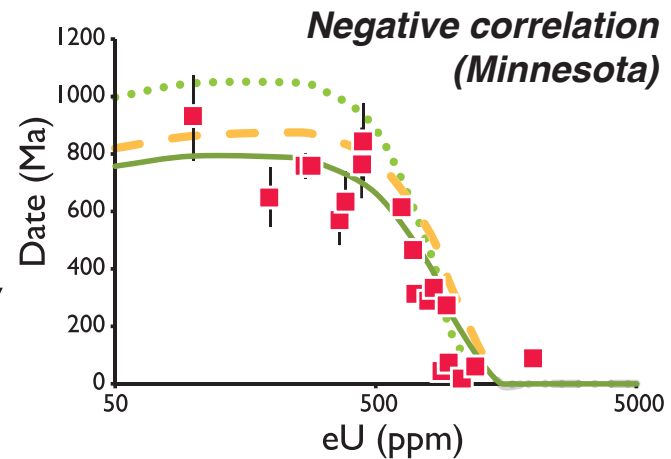
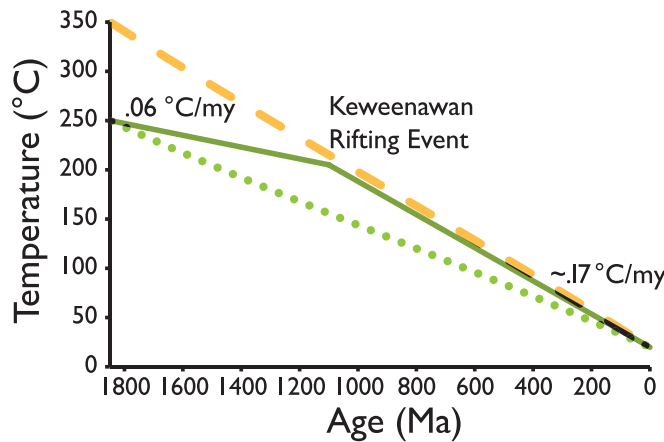
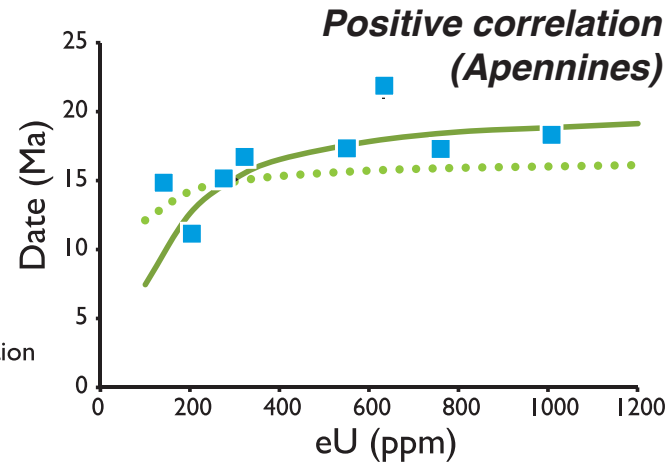
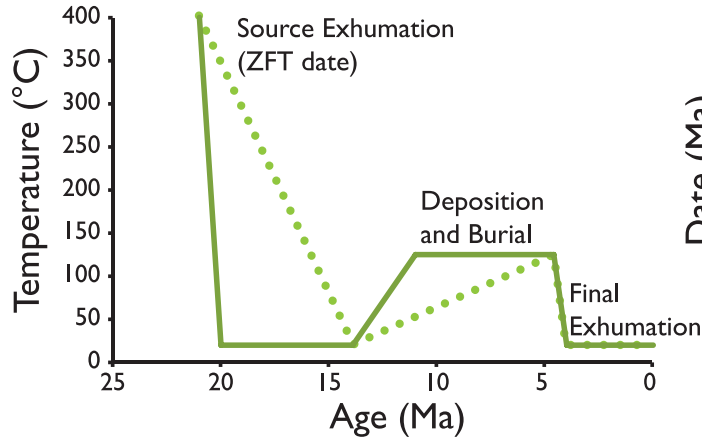
1. Strong modification of diffusion coefficient by recoil damage,
2. Damage clustering and interconnection
3. Lattice amorphisation at high dose



Guenther et al. (2013)

IV. Interpretation of ZHe data

Guenther et al. (2013)



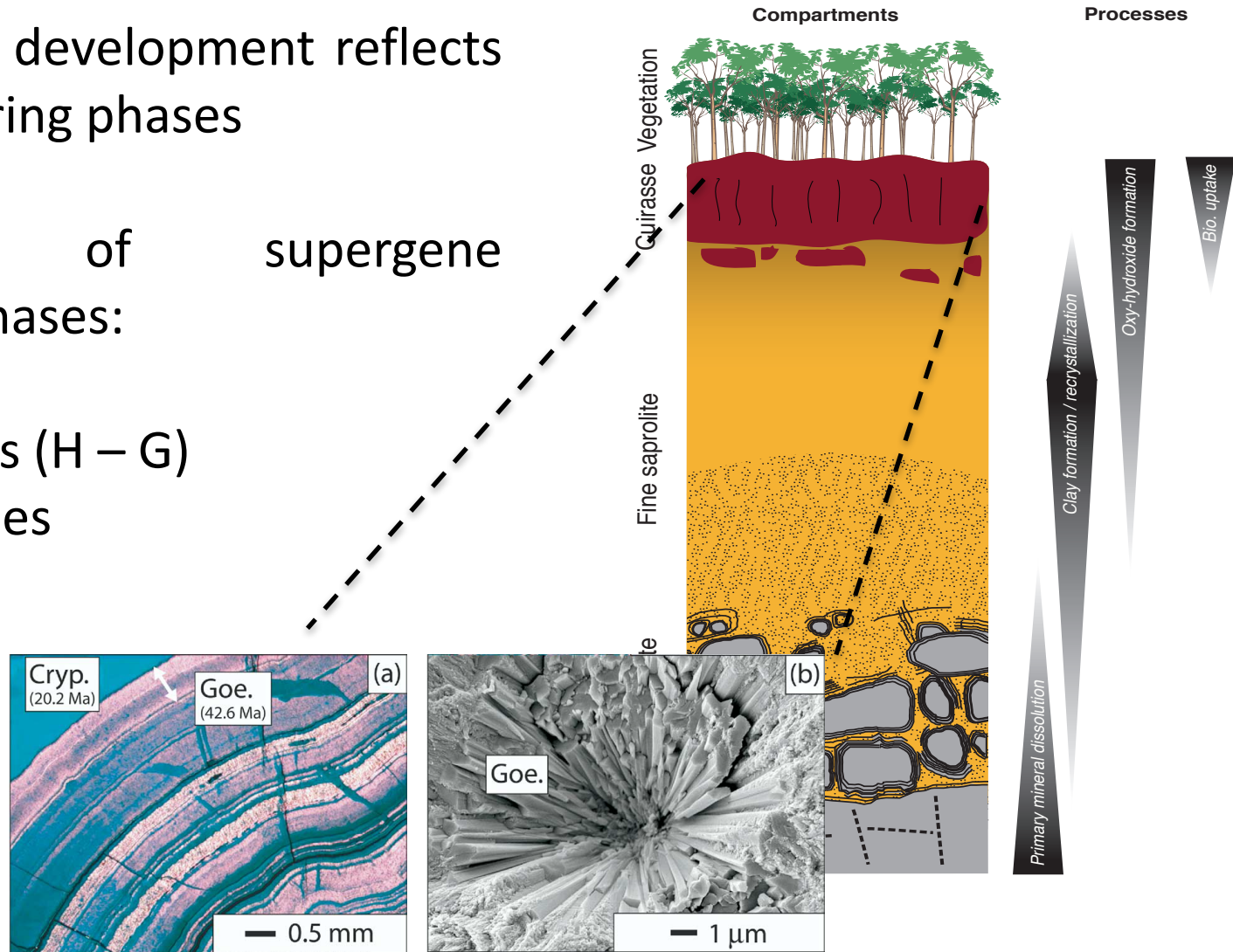
- Used of ZHe data dispersion to determine a precise thermal history, similarly to AHe

IV. Laterite, ore deposit dating

Laterite surface development reflects intense weathering phases

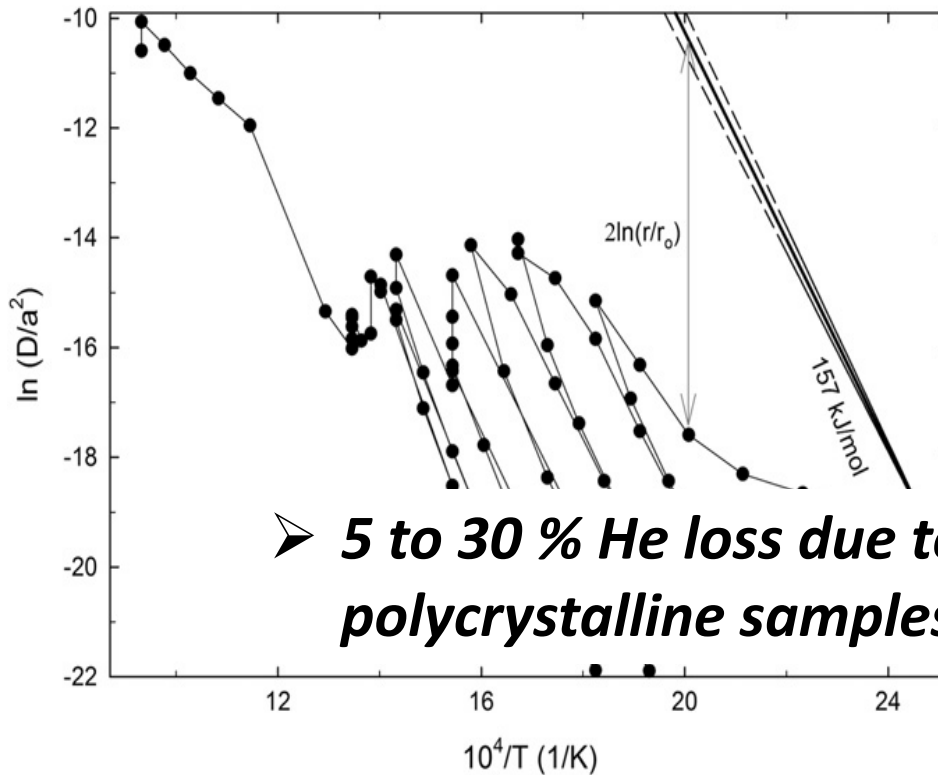
Crystallization of supergene mineralogical phases:

- Iron oxides (H – G)
- K-Mn oxides
- Kaolinites

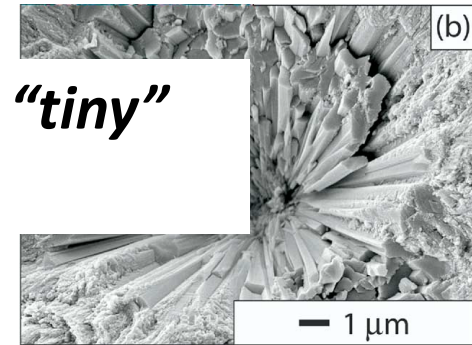
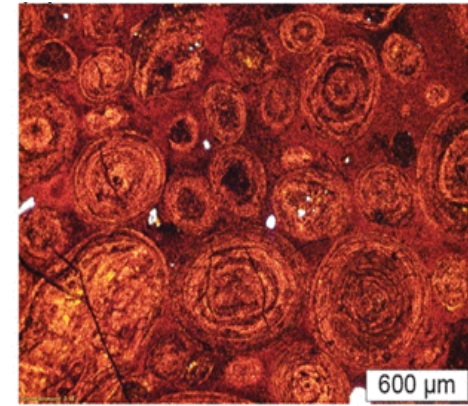


IV. Iron oxides

➤ He diffusion behavior in hematite and goethite



➤ **5 to 30 % He loss due to “tiny” polycrystalline samples**



➤ Crystals of 0.1 μm

Hematite

➤ $T_c(\text{He}) = 56^\circ\text{C}$

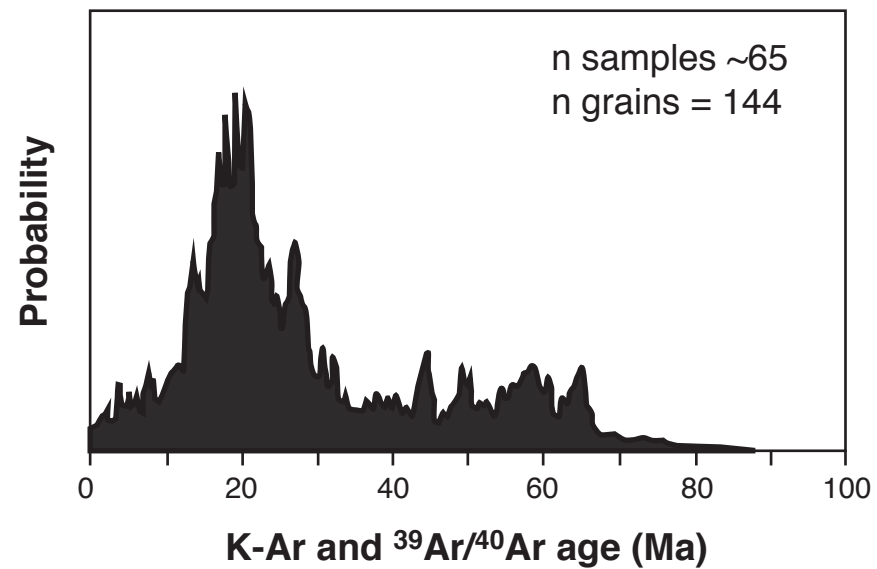
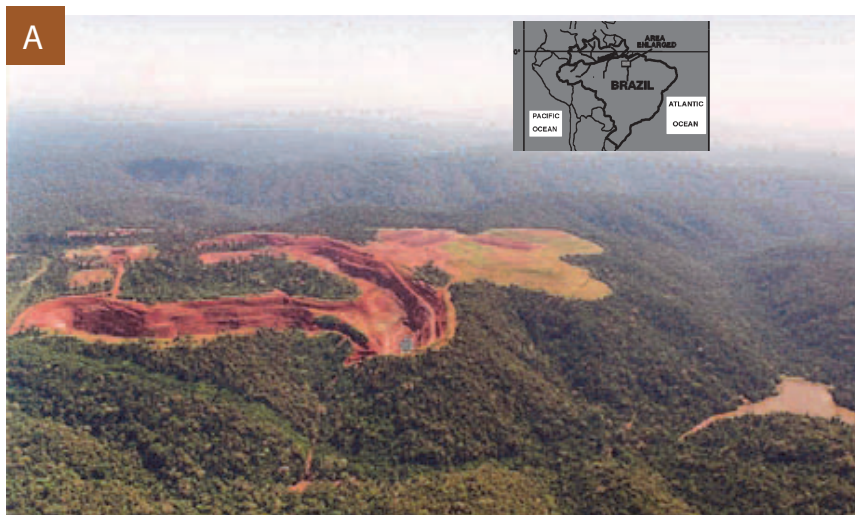
Goethite

➤ $T_c(\text{He}) \sim 49^\circ\text{C}$

*Shuster et al. (2005);
Farley and Flowers (2012);
Balout et al. (2017);
Allard et al. (Submitted)*

IV. Ore deposits

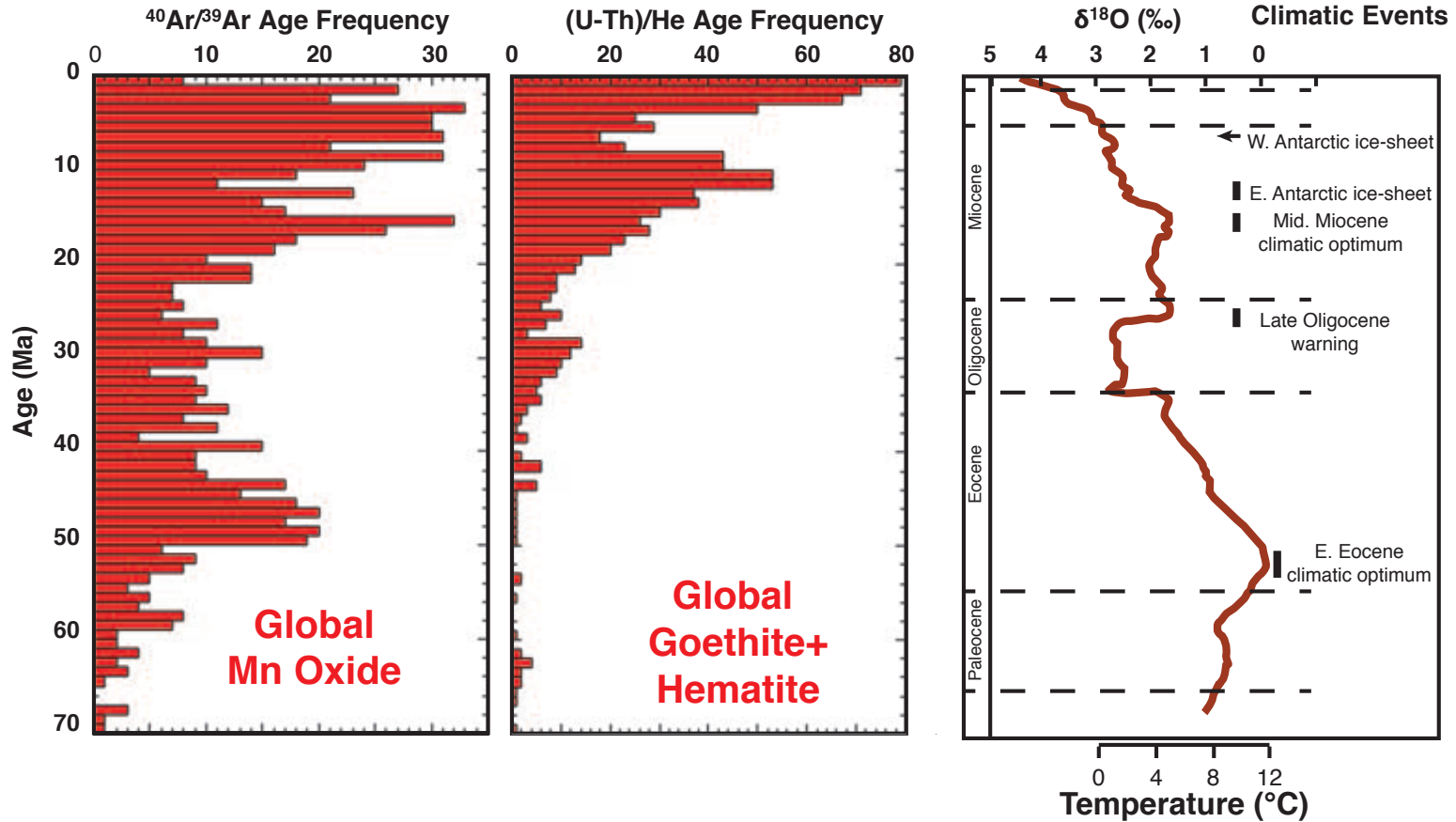
➤ Ore-deposit formation : Carajas Mountains (Brazil)



*Vasconcelos et al. (2015)
and references therein*

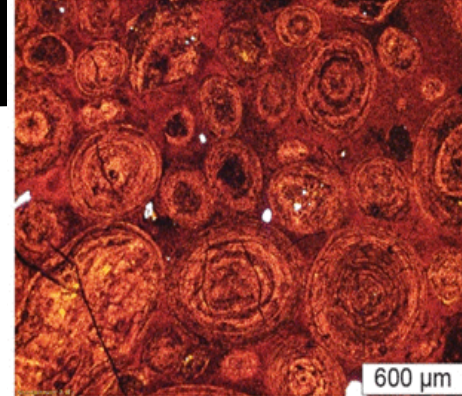
IV. Ore deposits

➤ All Amazonian and Australian laterites ages



Vasconcelos et al. (2015) and references therein

➤ Similar ages given by the K-Ar/Ar-Ar and (U-Th)/He systems



TAKE HOME MESSAGE :

(U-Th-Sm)/He dating can be applied to many systems if:

1. **Crystal contains U-Th-Sm AND**
2. **Produced He atoms are quantitatively retained in crystal lattice at surface temperatures (because of diffusion $\sim T_c > 40^\circ \text{C}$) AND**
3. **Grain or sample (made of polycrystalline grains) size are $> 100 \mu\text{m}$ (because of significant alpha ejection) AND**
4. **Possible strong damage impact on crystal lattice**

(1) (U-Th)/He dating system

I. Introduction, generalities

II. (U-Th)/He principles (chronometer vs thermochronometer)

(2) How to get an (U-Th)/He age

(3) Applications

III. Apatite (U-Th-Sm)/He (AHe) method

IV. Other applications (zircon, iron oxides,...)

(4) Exercises (Tc, ejection, weight, Rs), thermal modeling

(4) Exercises

Different exercises using diffusion coefficient (or T_c), and notions seen during lecture: ejection, diffusion domain, age calculation and dispersion

- 1. Closure temperature calculation**
- 2. Alpha ejection, R_s , weight determination ($Q_{t_{flop}}$)**
- 3. AHe age simulation using HeFty**

(4) Ex 1. closure temperature calculation

- With the given D_0 and E_a , **calculate the closure temperature T_c** , for a given cooling rate and grain size (a)

E_a (kJ/mol)	139.5
D_0 (m²/s⁻¹)	3.37×10^{-2}

$$T_c = \frac{E_a}{R \ln \left(A \tau \frac{D_0}{a^2} \right)} \quad \tau = \frac{RT_c^2}{E_a T}$$

Dodson (1973)

- With $R=8.31$ J/mol/K; $A=55$ and $T=273$ K

(4) Ex 1. closure temperature calculation

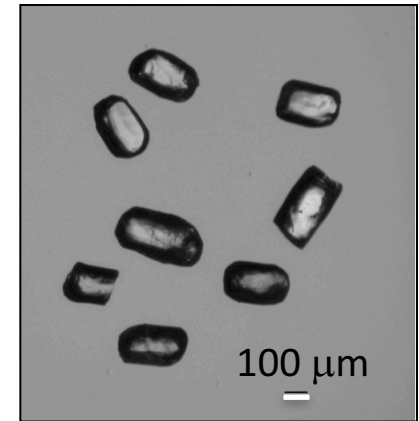
➤ Using an excel sheet, enter the need values need

	values	
Ea (J/mol)	139528,4	
D ₀ (m ² /s ⁻¹)	3,37E-02	
a (m)	1,70E-04	
D ₀ /a ²	1,17E+06	!! Values to change !!
R	8,31	
A (sphère)	55	T1 Temperature (°C)
T (°K)	345,00	72,00
		Cooling rate (°C/Ma)
Cooling rate (°/s)	3,17E-13	10
tau	2,24E+13	
Tc (°K)	345	
Closure temp Tc (°C)	71,66	When it's the same value of T1

conversion 1 cal => 4.18 J/mol

(4) Ex 2. grain characteristics

1. You have carefully selected apatite crystals and reported all measurements. Using those values, calculate the:
 - a. Apatite weight
 - b. R_s (equivalent diffusion domain)
 - c. F_T (ejection factor)



2. For one sample, you are not sure if the termination was 2 broken faces or no pyramids. Test the influence on the F_T factor.
3. Test the influence of **U-Th zonation** on the F_T factor.
4. Calculate the corrected AHe age and estimate the maximum age dispersion induced by the F_T factor (geometries, zoning) 79

(4) Ex 2. grain characteristics

➤ For grain measurement, you get the following data:

Name	Geometry	H (μm)	W (μm)	T (μm)	Weights (μg)	FT	Rs (μm)
Hel_1	2bf	200	125	115	6.8	0.83	64.8
Hel_2	1+1	160	125	115	4.2	0.80	59.8
Hel_3	No py	200	145	140	9.4	0.81	73.5
Hel-4	2 bf	150	80	70			


With:

2 bf=2 broken faces	1+1=1 pyramid + 1 bf
No py=No pyramids	

(4) Ex 2. grain characteristics

1. Selected the grain shape
2. Grain geometry
3. Grain size
4. Use a Th/U value
5. For zonation, selected where the U-Th content is localized and normalized amount and size.

Ketcham et al. (2011); Gautheron et al. (2012)



Alpha FT-ejection factor
Cecile Gautheron, Laurent Tassan-Got and Richard Ketcham

Inputs

Geometry

Grain list

Grain 1	Regular Hexagonal
Grain 2	1 pyramid

Radius (μm) 100.0
H (μm) 300.0

New Grain
Delete Grain
Clear List

Zonation

use zonation Number : 1

N°: 1 ratio: 0.00 size: 0.0

Medium

apatite
 Default density
Density (g/cm³) 3.1

Alpha List

Th/U
Th/U
1.0

MC

Number of events
1000000

Compute Help Quit

Results

He Range (μm):	20.33	Actual density (g/cm ³):	3.10
FT:	0.845	Mass (μg):	16.11
R_sph (μm):	90.7		

Ketcham et al., 2011, GCA, doi:10.1016/j.gca.2011.10.011
Gautheron and Tassan-Got, 2010, Chem. Geology, doi:10.1016/j.chemgeo.2010.02.023

Version date: 10/02/2012 based on Qt: <http://qt.nokia.com/>

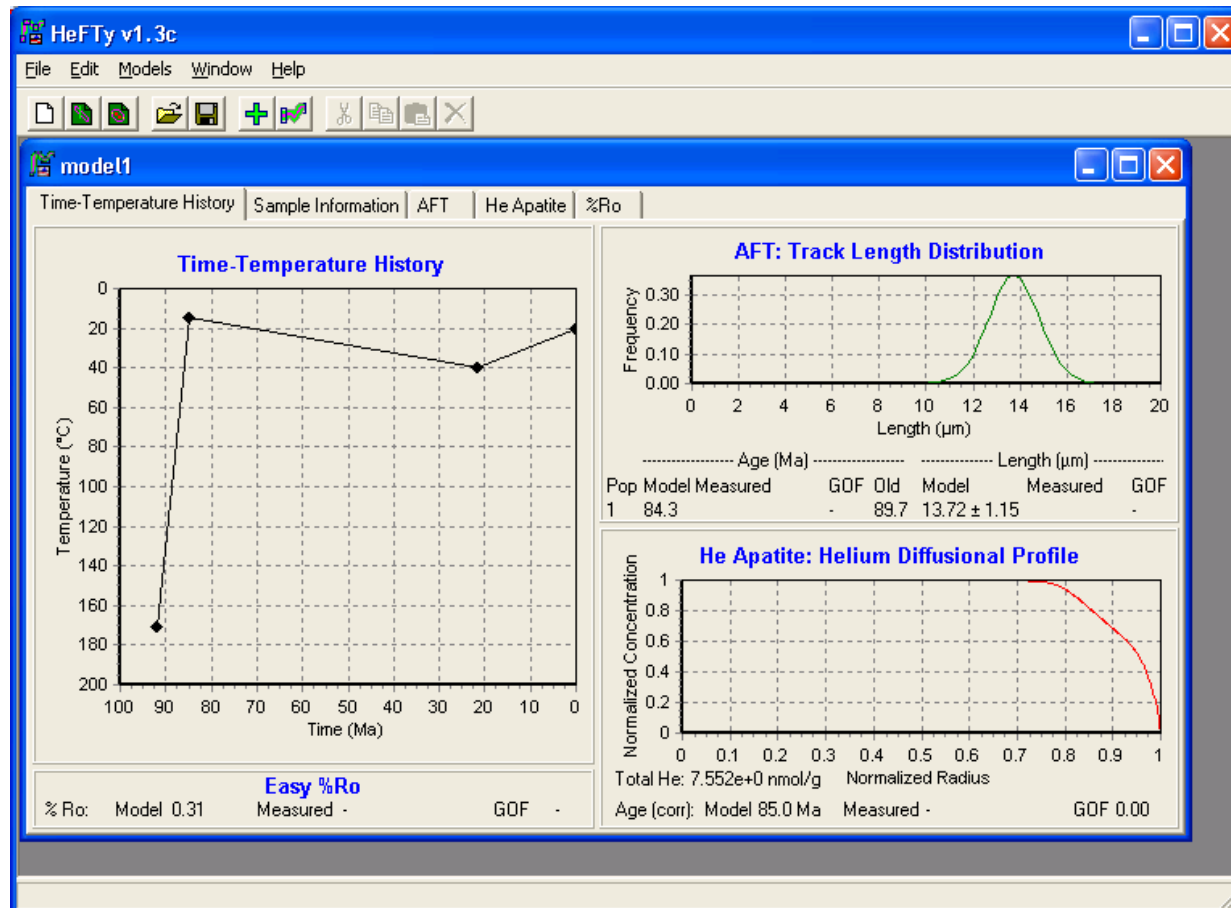
(4) Ex 2. grain characteristics

- With He, U, Th and Sm, you get the raw age for your sample.
 1. Calculate the alpha ejection corrected age
 1. Estimate the error on AHe age, by determining also the error associated with the determination of the F_T factor, knowing that the analytical error was at 4%.

Name	F_T	s	Rs	^4He	U	Th	Sm	eU	Th/ U	Raw age	Cor age	σ
			(μm)	(nmol/g)	(ppm)					(Ma)		
Hel_1	0.83	4%	64.8	2,21	17	61	296	31	3,7	12,2	14.7	8%
Hel_2	0.80	4%	59.8	34,19	103	265	383	167	2,6	37,4	46.7	8%
Hel_3	0.81	4%	73.5	0,11	1	4	275	2	4,8	4,8	5.9	8%

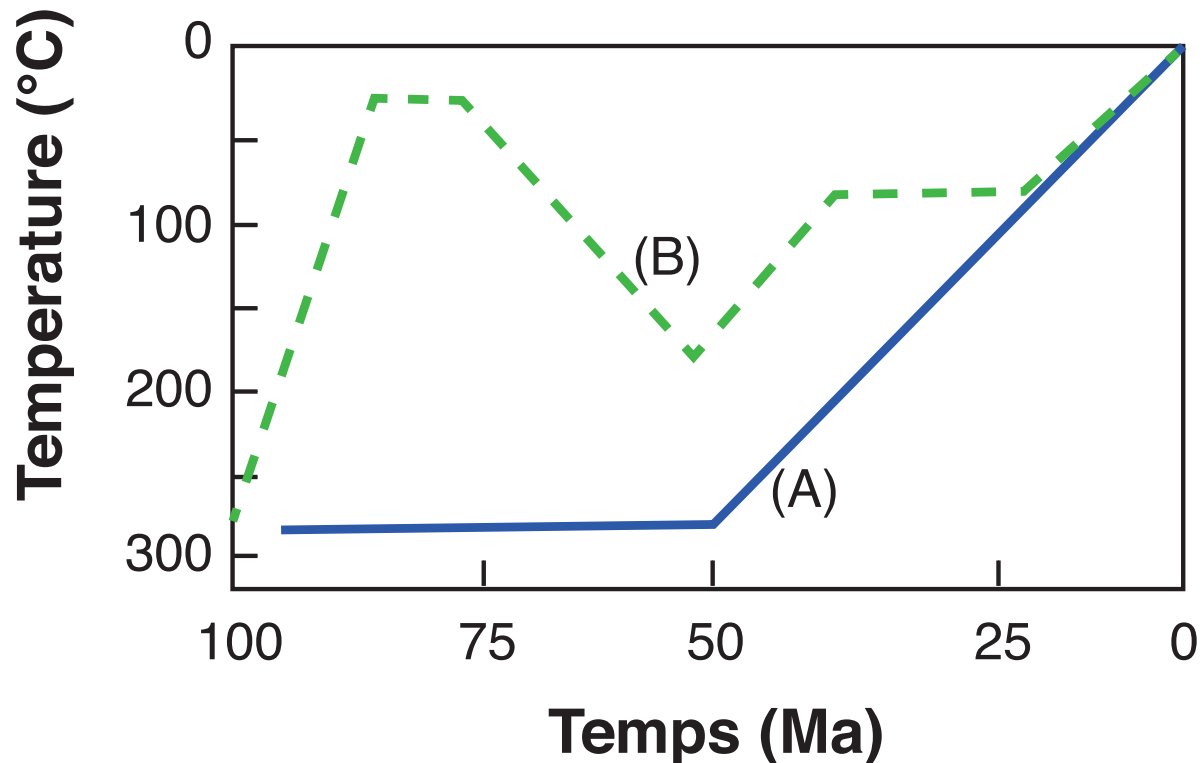
(4) Ex 3. AHe age simulation

1. Using HeFTy, we will simulate AHe, ZHe and AFT age distribution



(4) Ex 3. AHe age simulation

1. Test on AHe and ZHe age for two different thermal histories (A and B), the impact of:
 - a. Grain size,
 - b. eU content
 - c. grain chemistry (for apatite via the rmr_0)



Cited references

Cited references

- ✧ Balout, H., Roques, J., Gautheron, C., Tassan-Got, L., Mbongo-Djimbi, D., 2017. Helium diffusion in pure hematite (α -Fe₂O₃) for thermochronometric applications: a theoretical multi-scale study. *Computational and Theoretical Chemistry*, 1099: 21-28.
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