Mfront user day 2023

Microstructure-based modelling of snow viscoplasticity using FFT-based simulations and MFront to model crystal plasticity

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November 2023

Context: what is snow settlement?

T= 0 h

Winter storm in Virginia (USA) between January 22 and 24, 2016, adapted from WorseThanChiggers

Context: what is snow settlement?

T= 16 h

Winter storm in Virginia (USA) between January 22 and 24, 2016, adapted from WorseThanChiggers

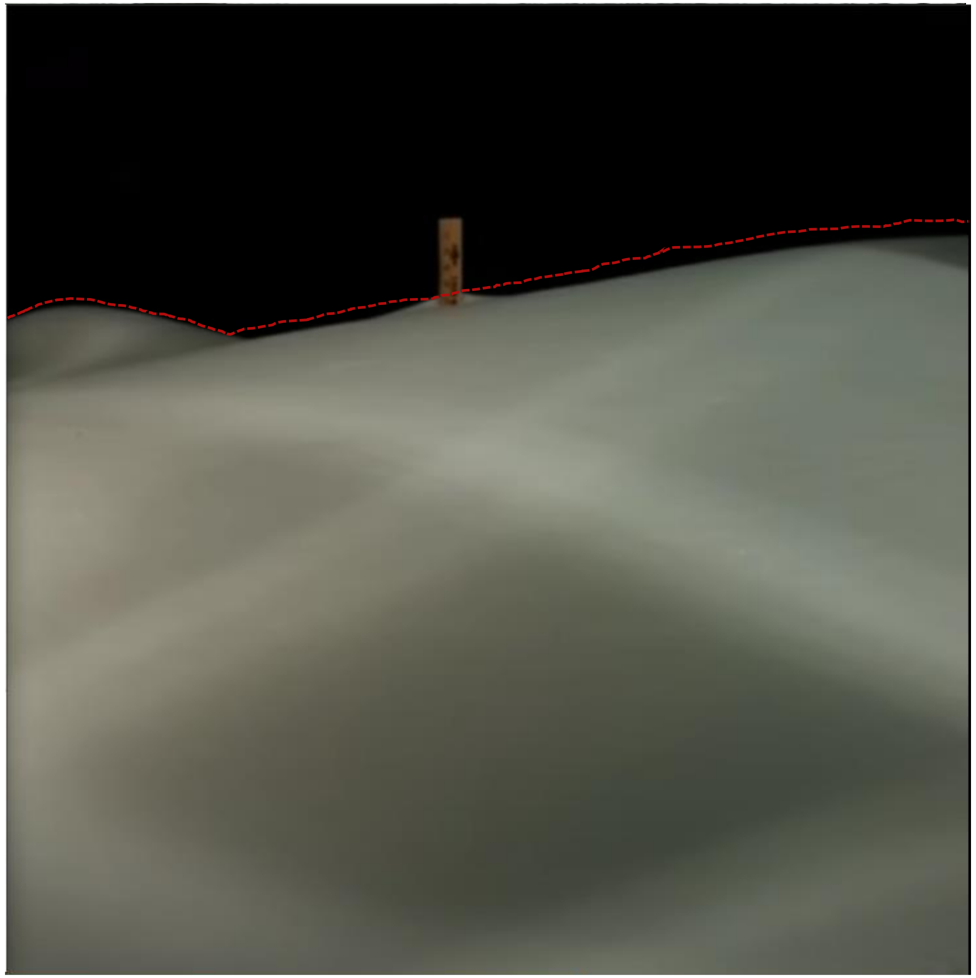
Context: what is snow settlement?

T= 35 h

Winter storm in Virginia (USA) between January 22 and 24, 2016, adapted from WorseThanChiggers

The snowflake that falls out of the sky doesn't stay that way for long…

Context: what is snow settlement?



T= 38 h

Winter storm in Virginia (USA) between January 22 and 24, 2016, adapted from WorseThanChiggers

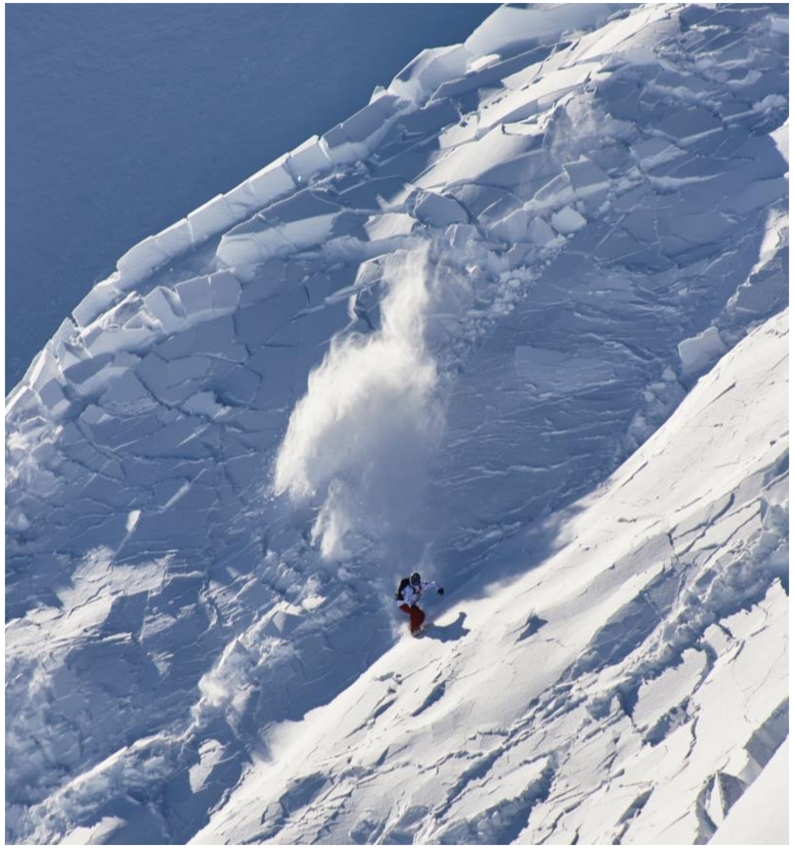
The snowflake that falls out of the sky doesn't stay that way for long

The snowflakes change their form and become more rounded

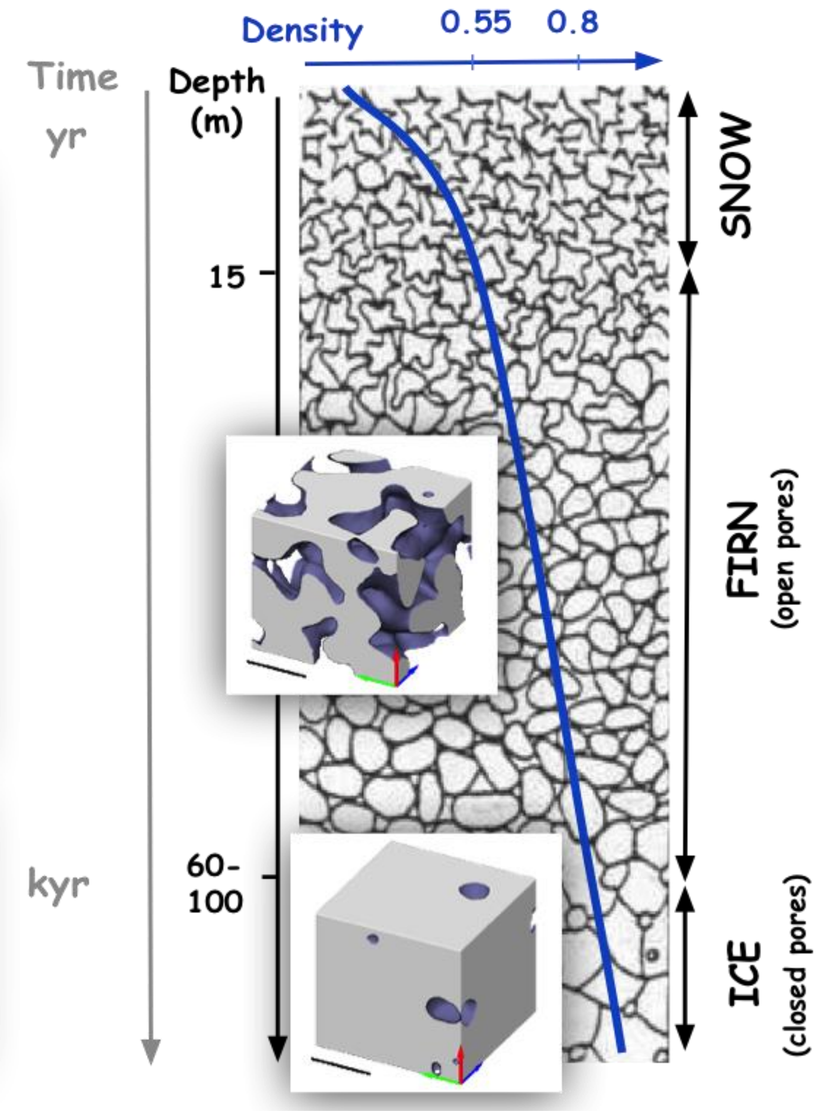
Settlement is the **slow** deformation of the snow as it densifies and sags under the influence of **gravity**

Context: applications

- Snowpack modelling, Paleoclimatology …



Snowboarder Mathieu Schaer. Credit: Ruedi Flueck



Schematic view of the snow-firn ice Continuum (Dumont et al., 2020)

Context: snow microstructure

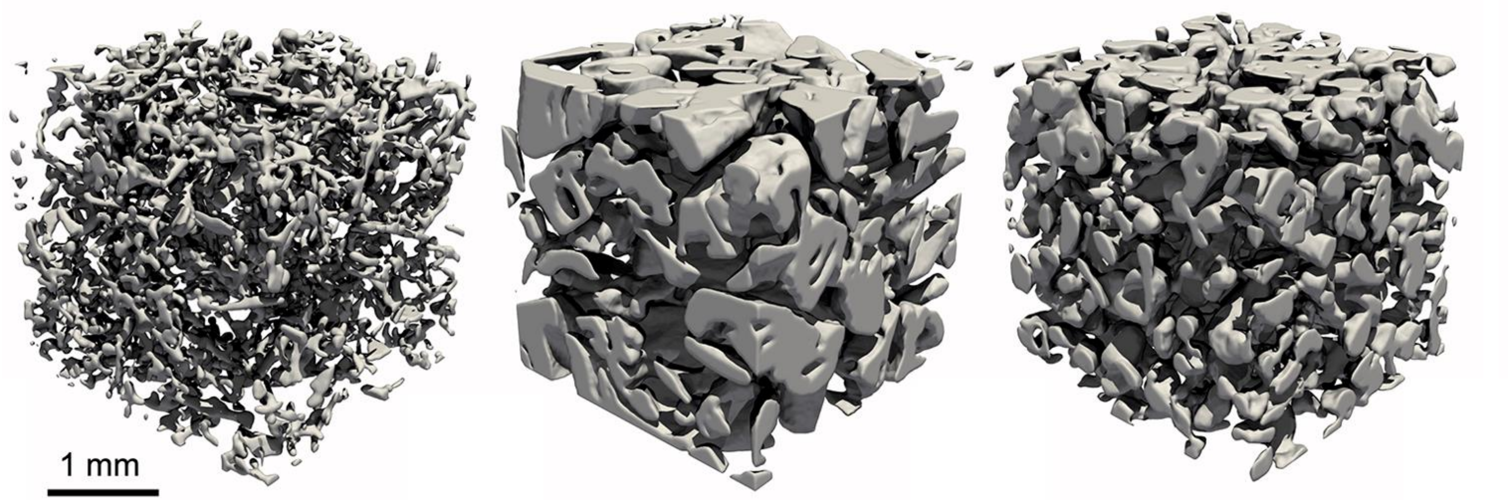
Snow = mixture of ice crystals sintered together, air and sometimes liquid water and impurities.

Material close to the melting temperature

Porosity → 95% fresh snow / 10% for dense firn

Large number of snow type → difficult to characterize

Snow settlement is mainly driven by the creep of the **ice matrix** undergoing **viscoplastic deformations**



Three-dimensional view of the microstructure of some representative snow samples. Measured with X-ray microtomography by Lin et al., (2022).

Cup-shaped crystals in the snowpack (SLF).

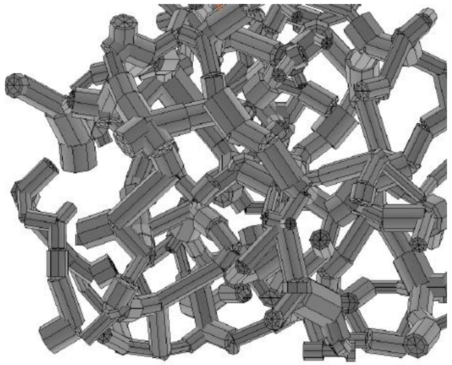
Scientific questions:

- How does the viscoplastic behaviour of ice scales to the snow mechanical behaviour?

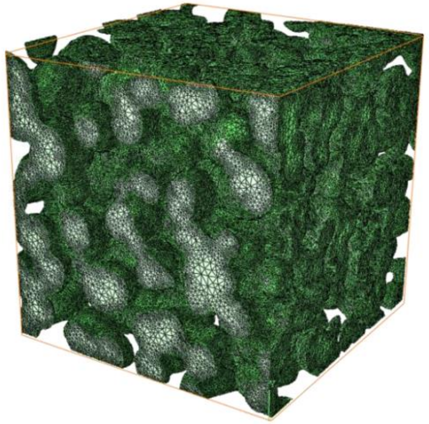
Key bibliography:

Investigation through microstructure-based simulations :

snow = 3D microstructure + ice mechanical properties



- *Theile et al., (2011):* highly simplified snow microstructure
  + advanced modelling of ice mechanics



- *Wautier et al., (2017):* faithful microstructure
  + rough ice mechanics

Scientific questions:

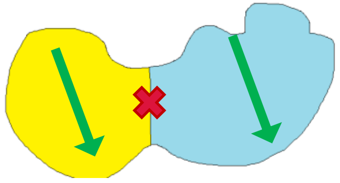
- How does the viscoplastic behaviour of ice scale to the snow mechanical behaviour?

Our work:

- Microstructure-based simulation: faithful microstructure + advanced ice mechanics, made possible via a suitable solver: AMITEX
- Direct evaluation based on previous creep experiments captured by tomography.

Contours of the study:

- Study of dry snow only, under isothermal conditions without metamorphism ;
- Account only intra-crystalline deformation (inter-crystalline sliding is overlooked).



Methodology:
experimental setup

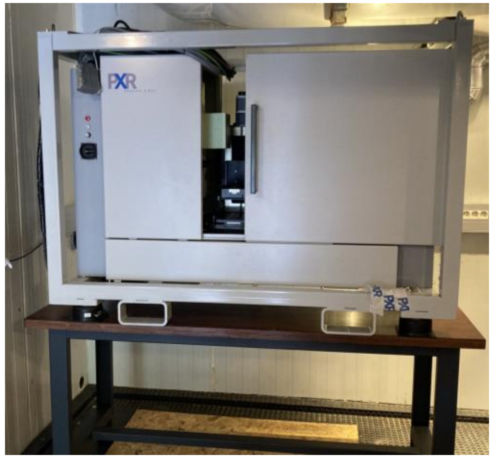
As our model **cannot reproduce the evolution of the microstructure**, we use the **set of experimentally obtained microstructures** to decompose the test into a set of instantaneous creep experiments.

We use two mechanical tests performed by *(Bernard et al., 2022):*

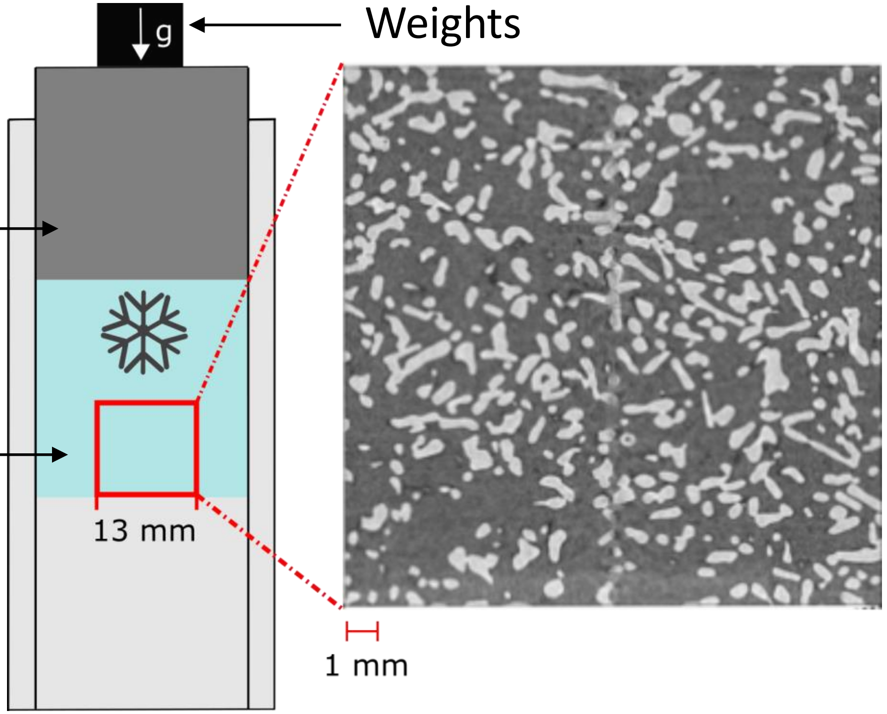
I) Load-controlled test:

- $\sigma_{imp} = 2.1$ kPa, $T_{snow} = -8 \pm 0.5$ °C
- Deformation determined based on density measurement

(X-Ray tomography)



Tomograph (Hagenmuller)



Experimental setup (Bernard et al., 2022)

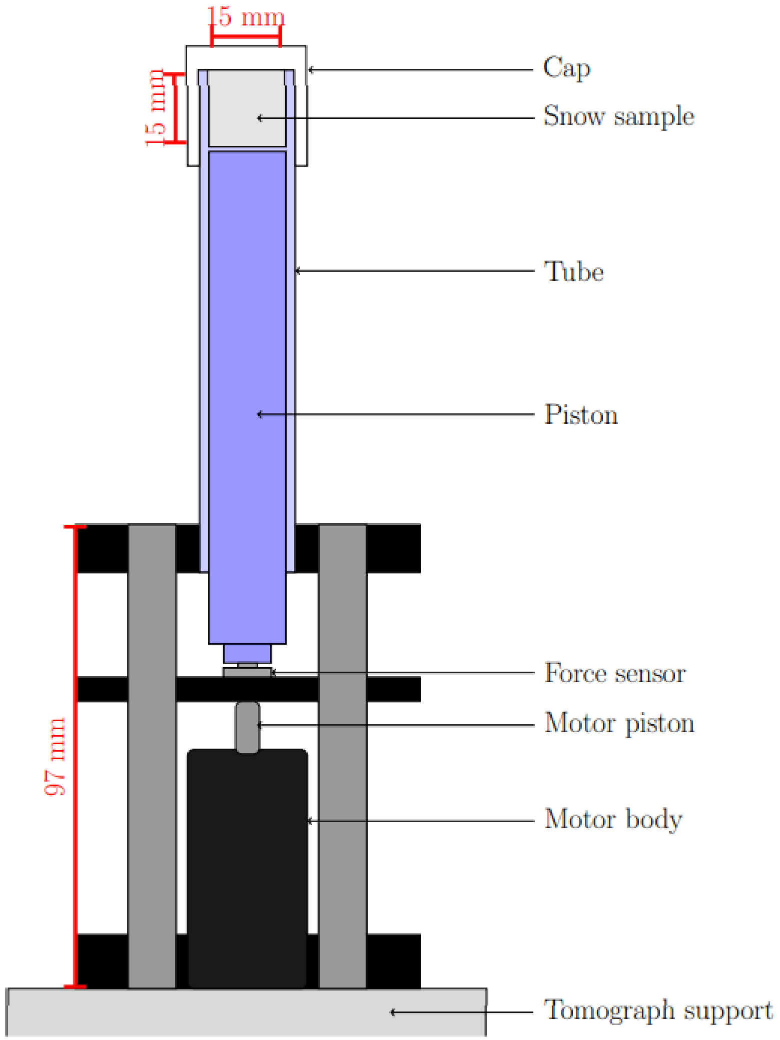
Methodology:
experimental setup

As our model **cannot reproduce the evolution of the microstructure**, we use the **set of experimentally obtained microstructures** to decompose the test into a set of instantaneous creep experiments.

We use two mechanical tests performed by *(Bernard et al., 2022-2023):*

II) Strain-rate-controlled compression test:

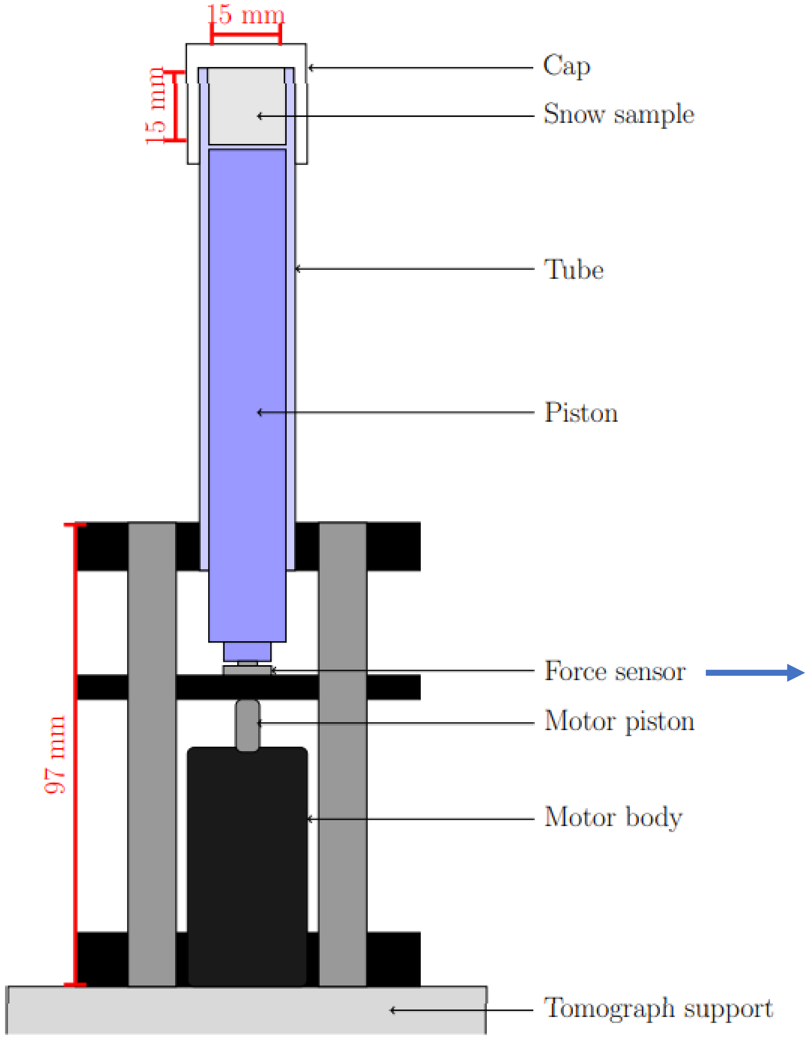
- $\dot{\varepsilon}_{\text{imp}} = 1.8 \times 10^{-6}\ \text{s}^{-1}$,
- $T_{\text{snow}} = -18 \pm 0.5\ °\text{C}$



Experimental setup (Bernard et al., 2023)

Methodology:
experimental setup

Strain-rate-controlled compression test



Allows to calculate the stress

Experimental setup (Bernard et al., 2023)

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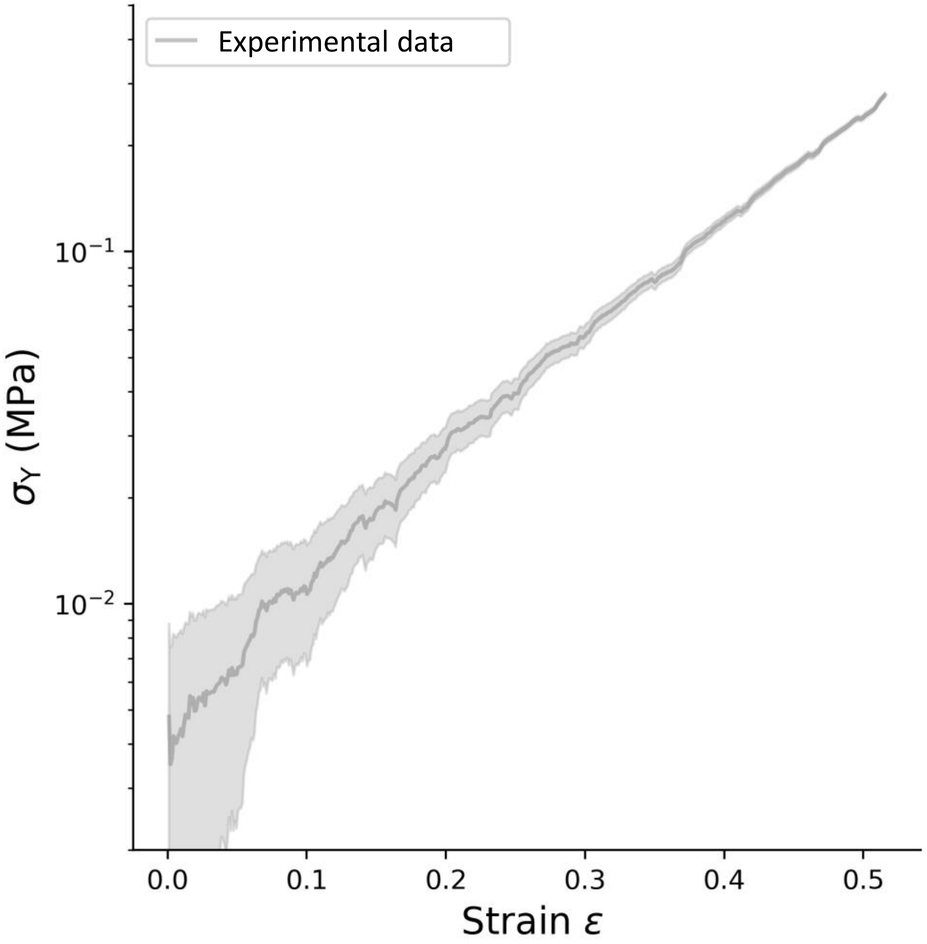
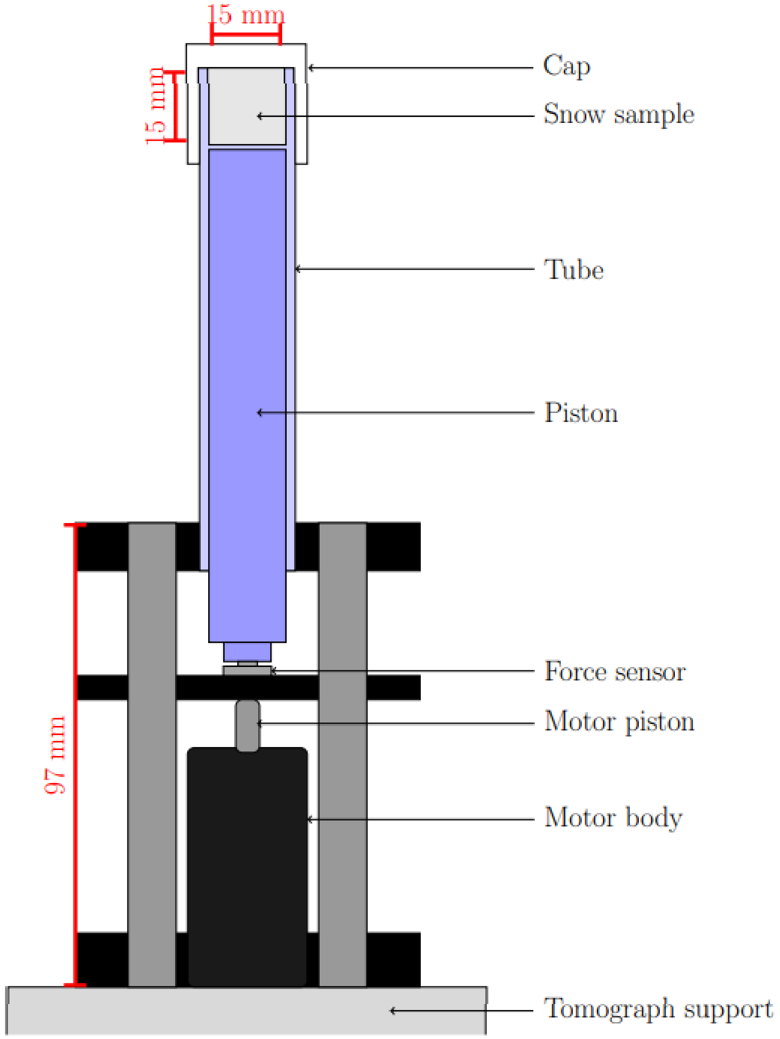
Methodology:
experimental setup



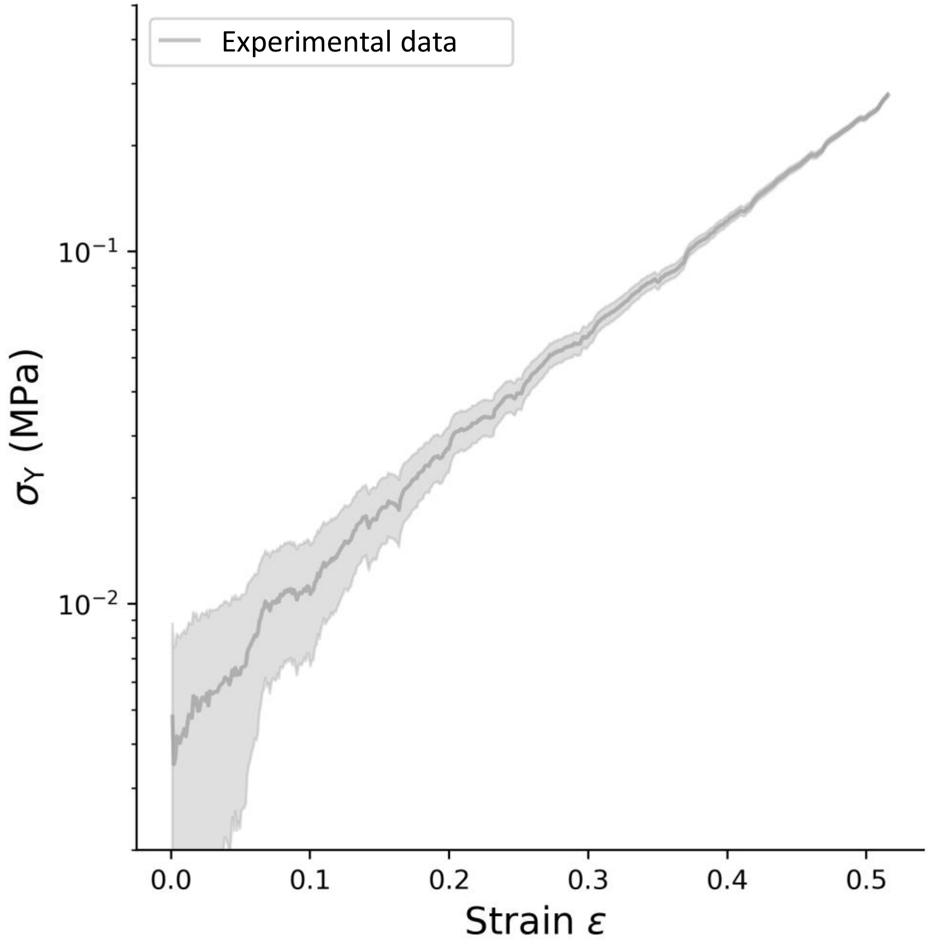
Strain-rate-controlled compression test

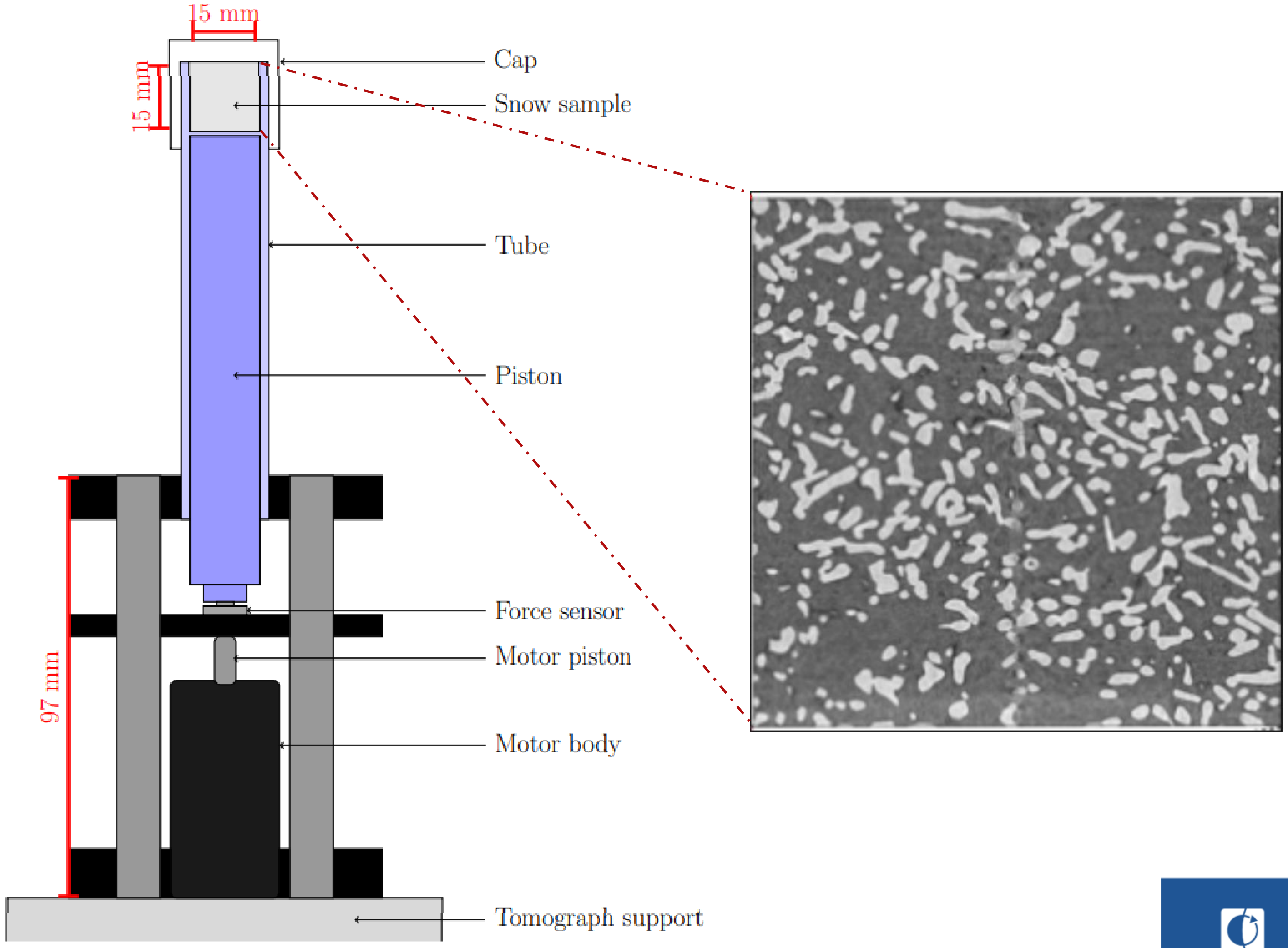


Experimental setup (Bernard et al., 2023)

Methodology:
experimental setup

Strain-rate-controlled compression test

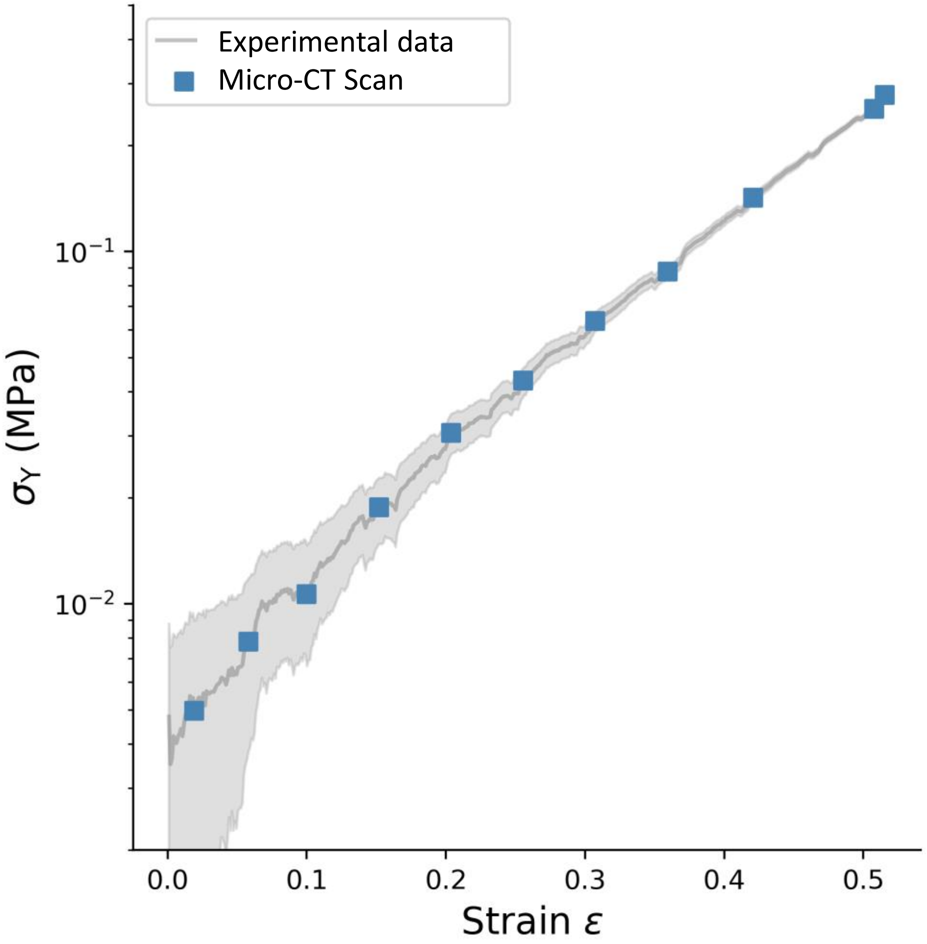


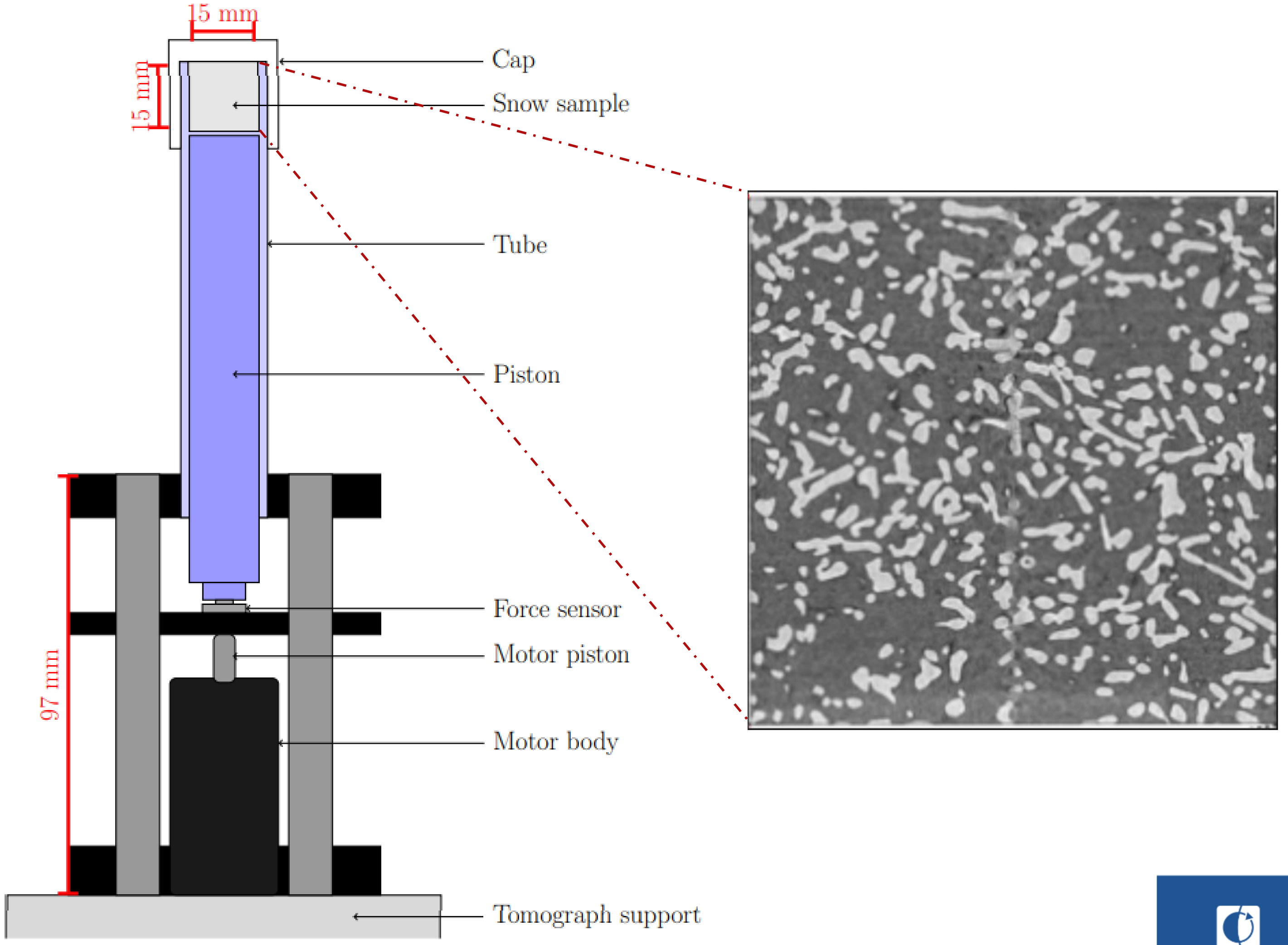


Experimental setup (Bernard et al., 2023)

Methodology:
experimental setup

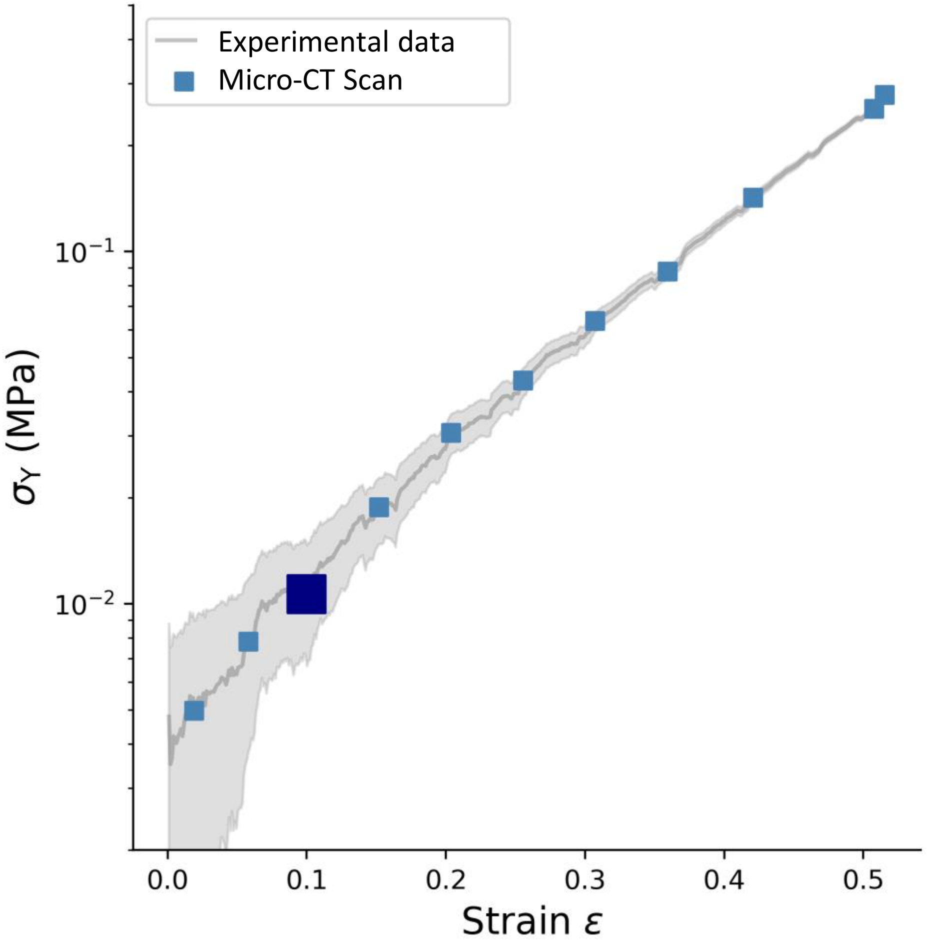
Strain-rate-controlled compression test



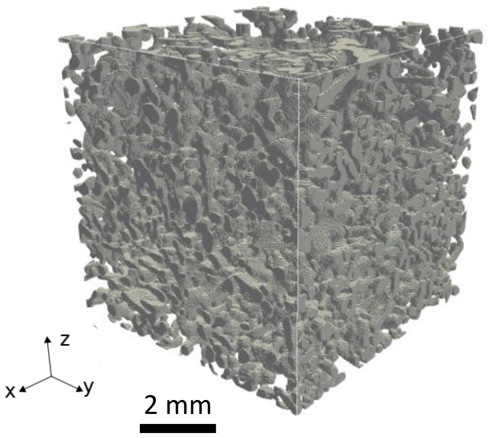


Experimental setup (Bernard et al., 2023)

Methodology:
numerical setup



Binary segmentation



Homogeneous ice model
3D Norton law *(Suquet, 1983)*

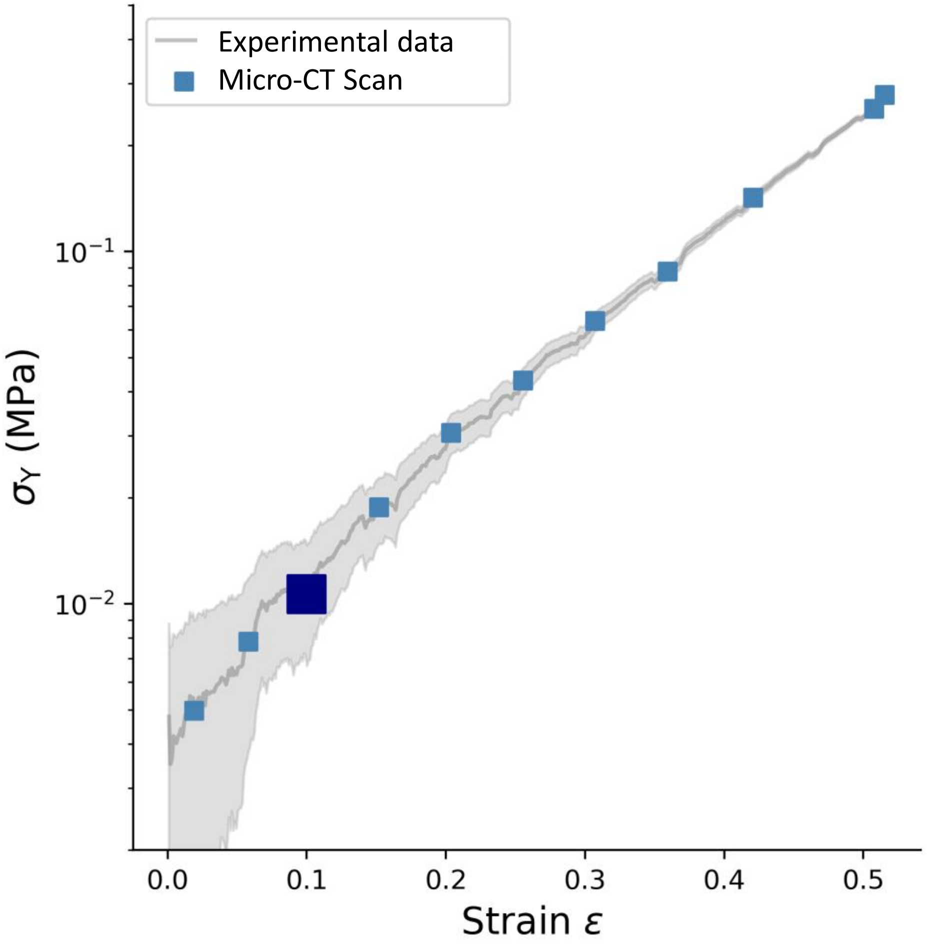
$$\epsilon = \epsilon_{\mathrm{e}} + \epsilon_{\mathrm{vp}}$$

$$\dot{\boldsymbol{\epsilon}}_{\mathbf{vp}} = \frac{3}{2} A\, \sigma_{\mathrm{eq}}^{n-1}\, \boldsymbol{\sigma}'$$

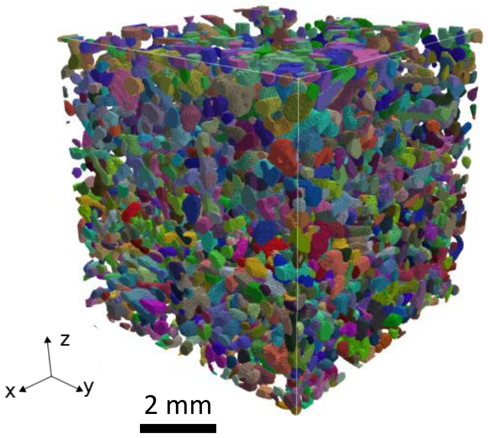
with σ_{eq} the equivalent stress, $\boldsymbol{\sigma}'$ the deviatoric stress, $A = 7.8\ 10^{-8}\ \mathrm{MPa}^{-\mathrm{n}}\ \mathrm{s}^{-1}$ and $n = 3$

From *Castelnau et al., 1998, Theile et al., 2011*

Methodology:
numerical setup



Grain segmentation



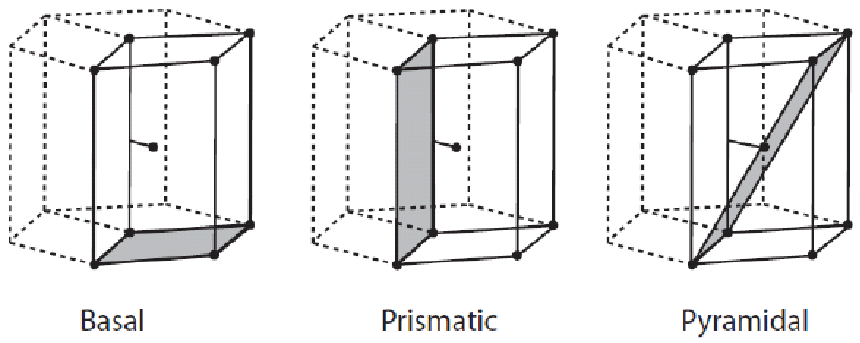
Sintered crystal model
Crystal plasticity

$$\boldsymbol{\epsilon}_{vp} = \sum_{k=1}^{12} \gamma^{(k)} \boldsymbol{\mu}^k$$

$\boldsymbol{\mu}^k = \frac{1}{2}(n^k \otimes_s b^k)$ the Schmid tensor

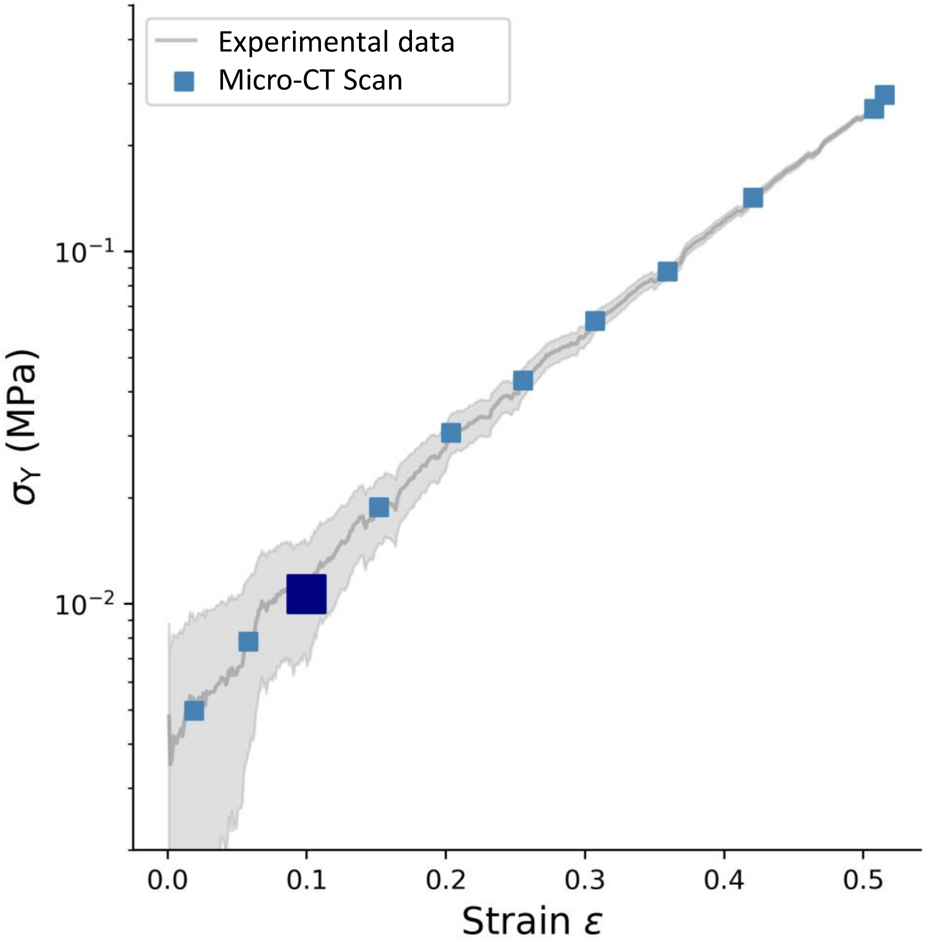
$$\dot{\gamma}^{(k)} = \dot{\gamma}_0^{(k)} \left(\frac{\left|\tau^{(k)}\right|}{\tau_0^k} \right)^{n^{(k)}} \operatorname{sgn}\left(\tau^{(k)}\right) \quad \text{with} \quad \tau^{(k)} = \boldsymbol{\sigma} : \boldsymbol{\mu}^{\boldsymbol{k}}$$

with $\tau_0^{(k)}$ the reference resolved shear stress,
$\dot{\gamma}_0^{(k)} = 1\ \mathrm{s}^{-1}$ the reference shear rate



The three slip systems present in ice crystal (Poerschke, 2009)

Methodology:
numerical setup



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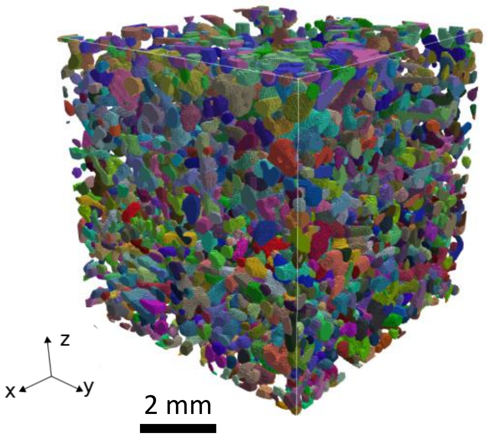

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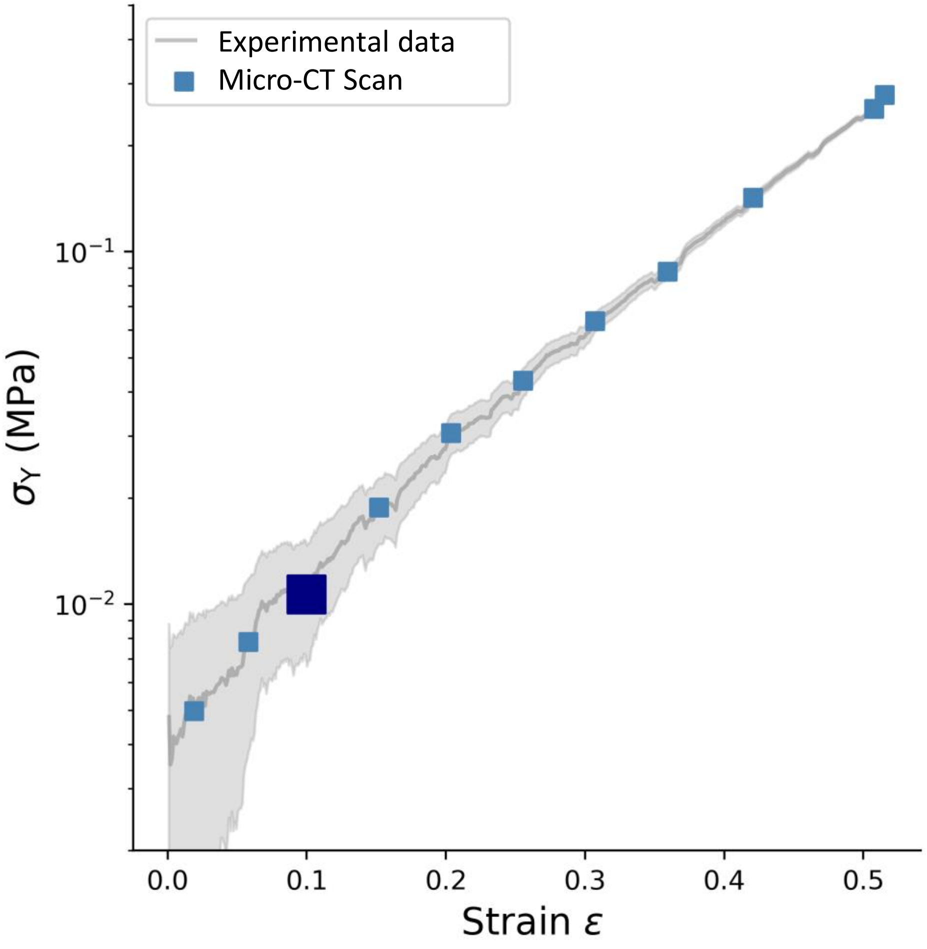
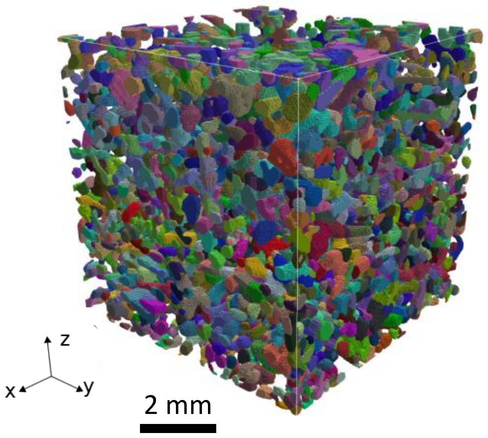
Family	Systems	$n^{(k)}$	$\tau_0^{(k)}\ (MPa)$
Basal [0001]<11$\bar{2}$0>	3	3	13
Prismatic [01$\bar{1}$0]<2$\bar{1}\bar{1}$0>	3	3	260
Pyramidal [11$\bar{2}$2]<11$\bar{2}\bar{3}$>	6	3	260

Monocrystalline ice parameters of viscoplastic model at −10 °C adapted from Lebensohn et al., 2009 and Hondoh, 2000

Methodology:
numerical setup



Grain segmentation



Sintered crystal model
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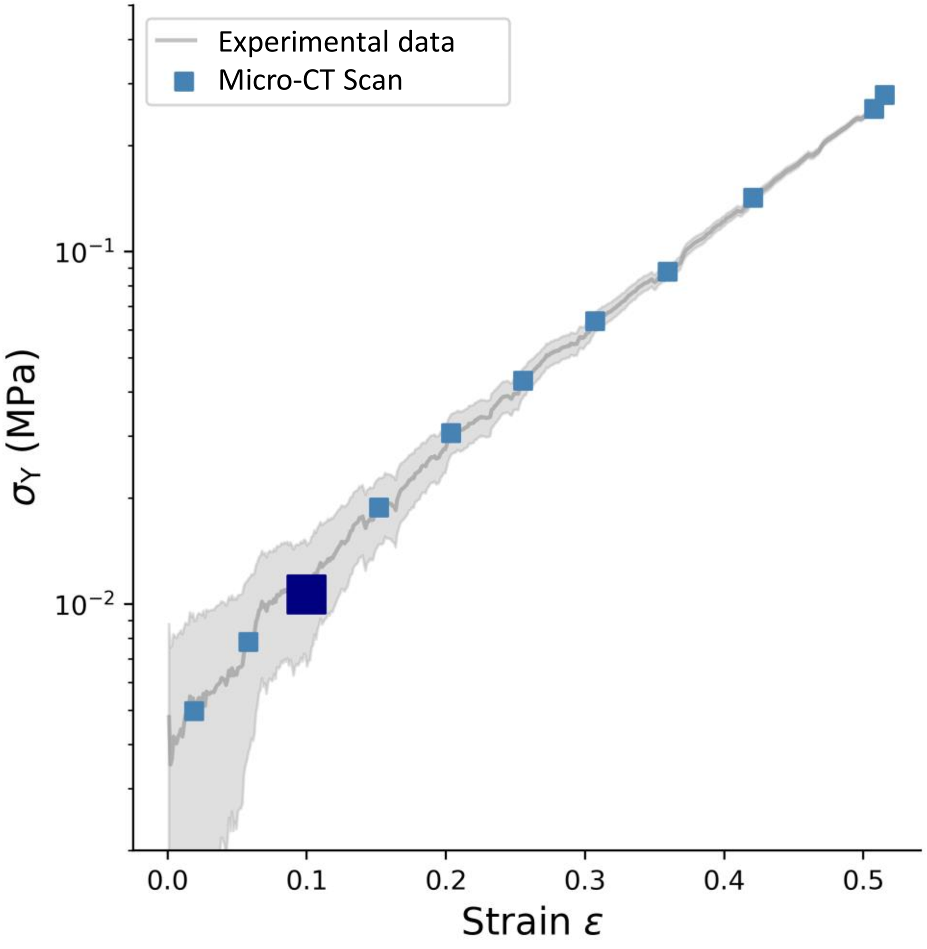
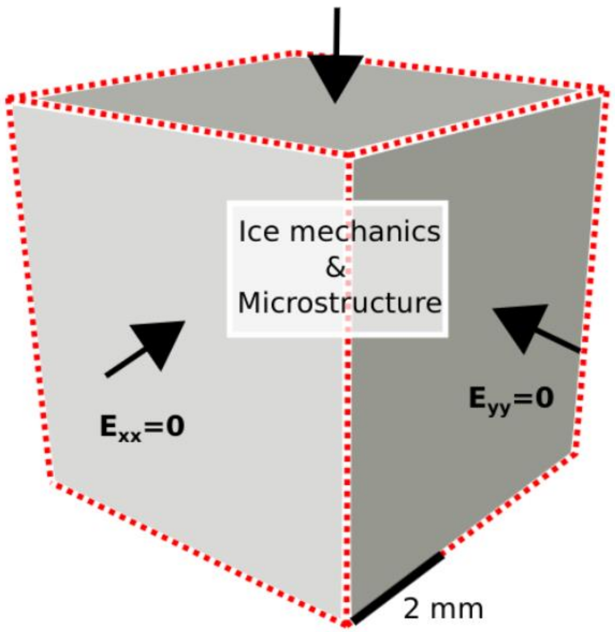
with $\tau_0^{(k)}$ the reference resolved shear stress,
$\dot{\gamma}_0^{(k)} = 1\ \mathrm{s}^{-1}$ the reference shear rate

→ Implemented with the *StandardElastoViscoPlasticity* brick (Helfer et al., 2019)

Methodology:
numerical setup



$$\mathbf{E_{zz}} = \mathbf{\dot{E}_{zz\,imp}}\, \boldsymbol{t}$$



Hypothesis no lateral friction:

$$\mathbf{\Sigma_{xy}} = \mathbf{\Sigma_{yz}} = \mathbf{\Sigma_{xz}} = \mathbf{0}$$

Use **AMITEX**

(Gélébart et al.,2020)

→ Voxel images are the direct input of the simulations

→ Benefits from the MPI parallelisation

Simulations on a Representative Elementary Volume (REV)

$5.1 \times 5.1 \times 5.1\ \mathrm{mm}^3$

as $L_{macro} \gg L_{micro}$

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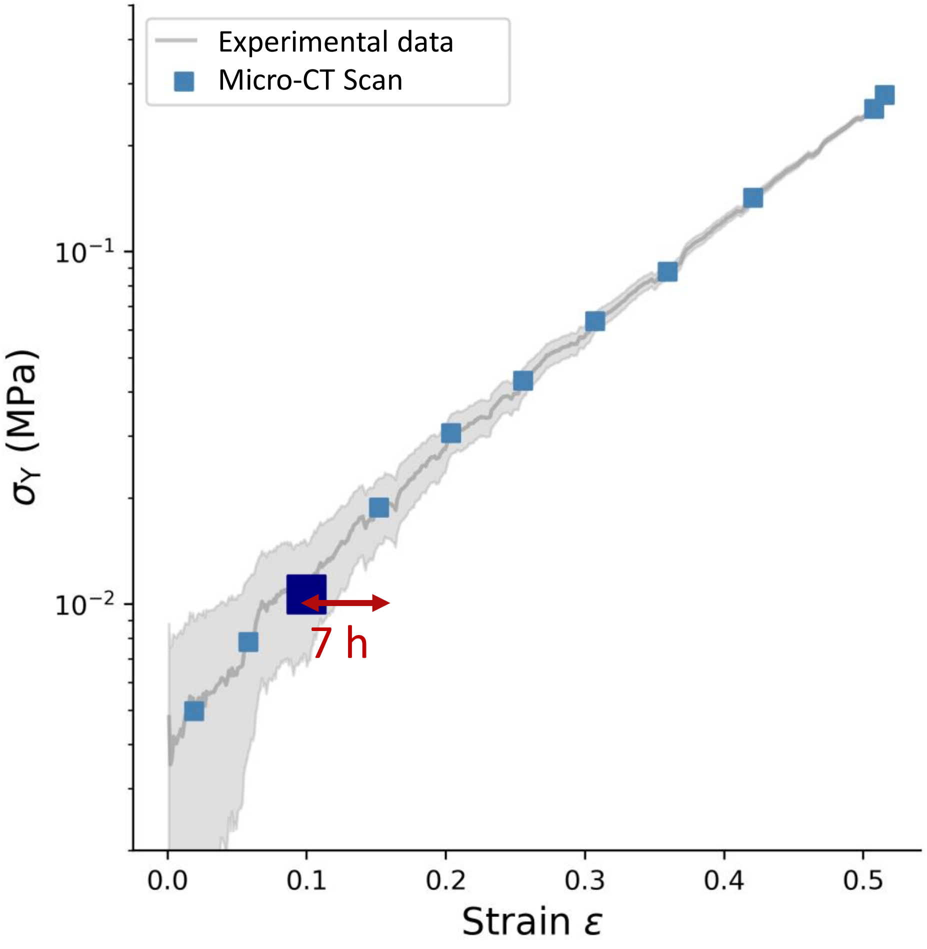
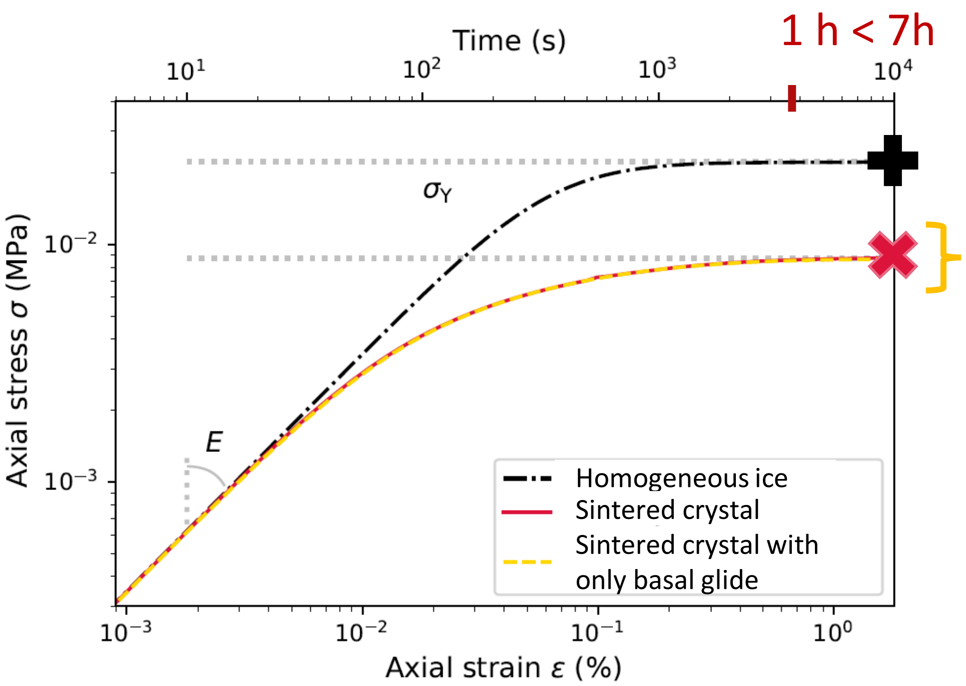
Results: compression tests



"instantaneous creep experiment "
topological changes negligeable



The basal mode is sufficient to represent snow creep.

Stress evolution with the strain for the different ice models.

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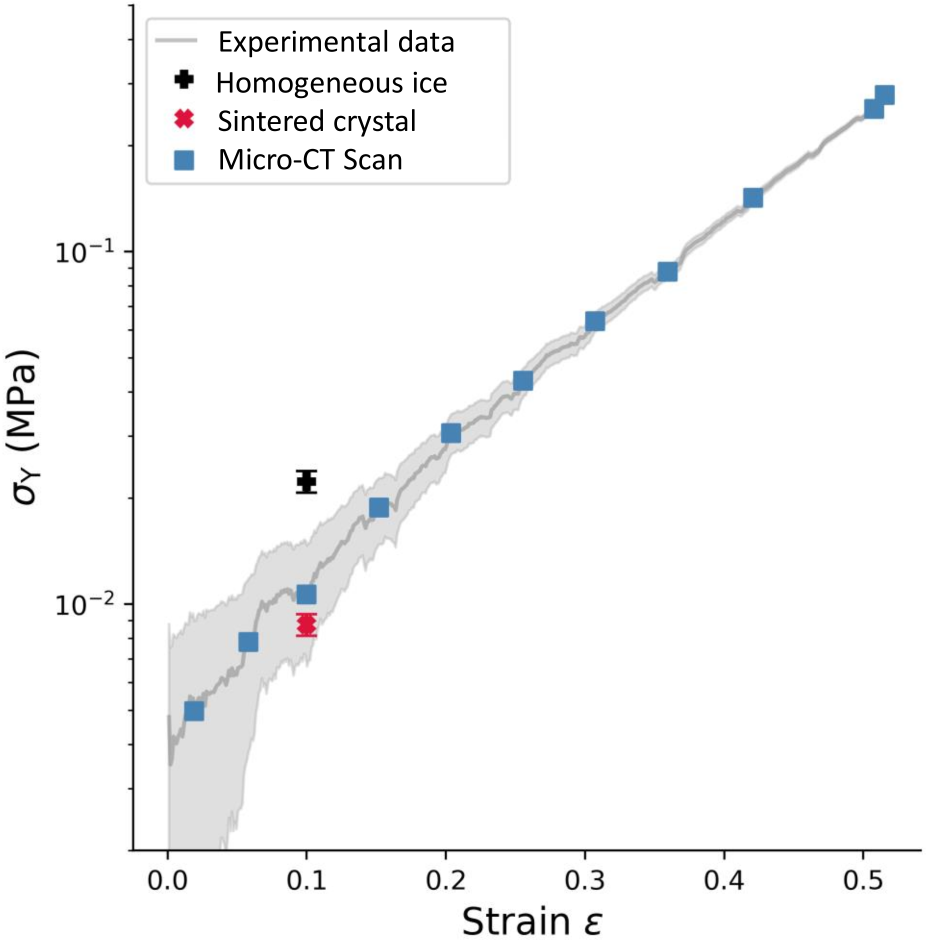
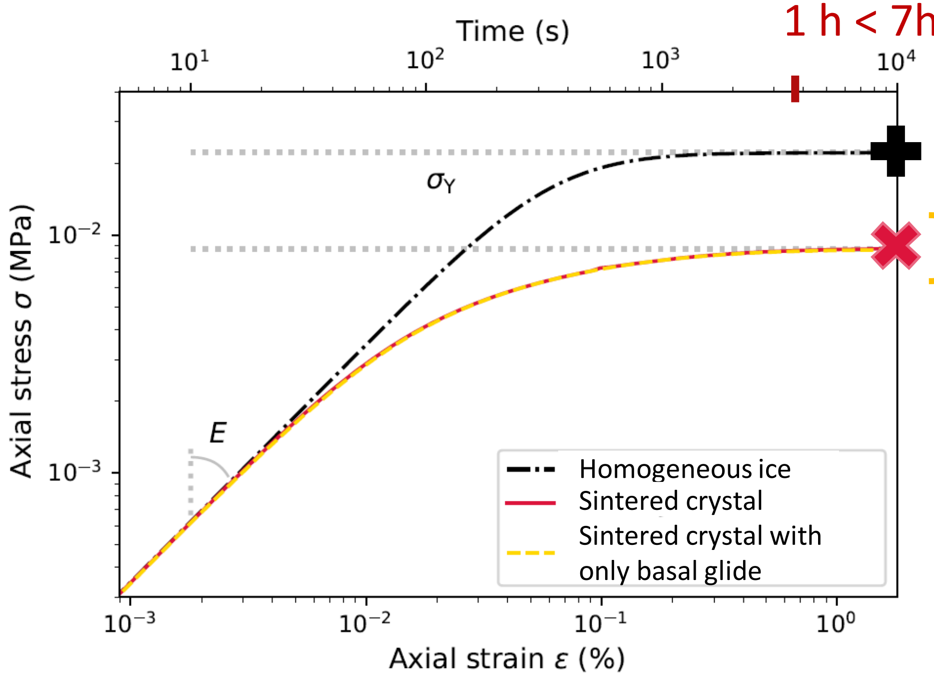
Results: experimental comparison



"instantaneous creep experiment "
topological changes negligeable

1 h < 7h



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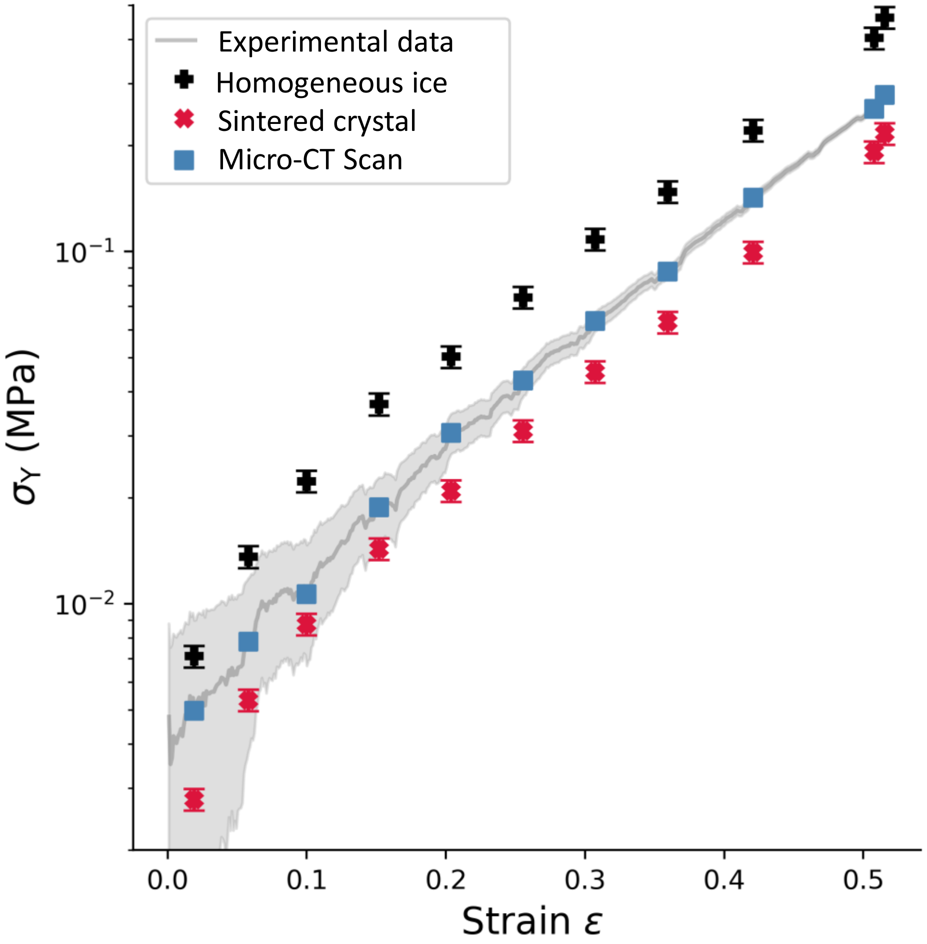


The same method is repeated for each scan …

Study of the nonlinear viscosity:

$$B = \frac{\sigma^n}{\dot{\epsilon}}$$

with *n=3* by homogeneization (*Wautier et al., 2017*)

The same process is repeated for the **load-controlled test**

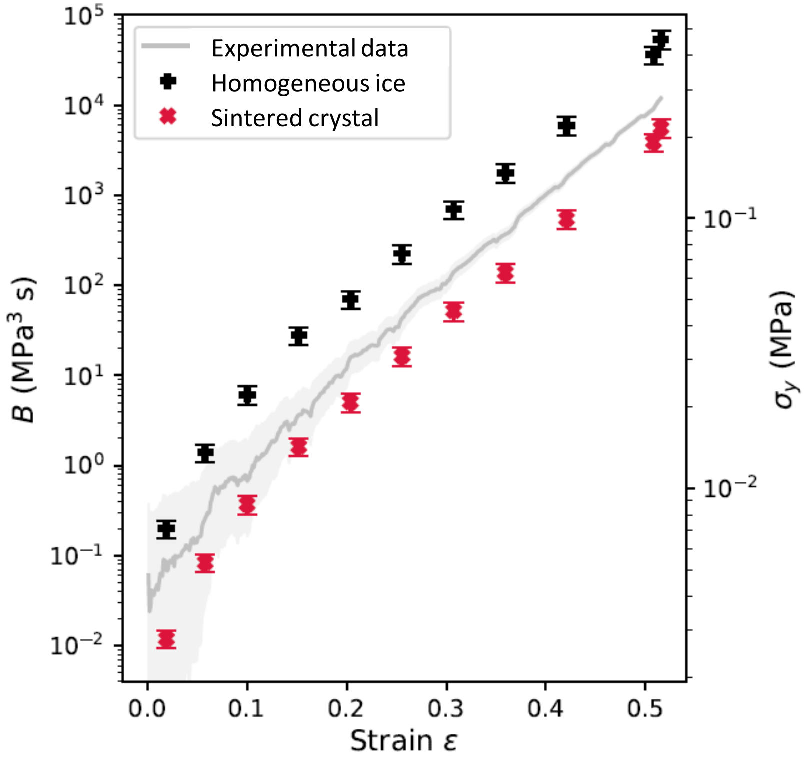
Results: experimental comparison

- Ice in snow should not be considered as a foam of ice,

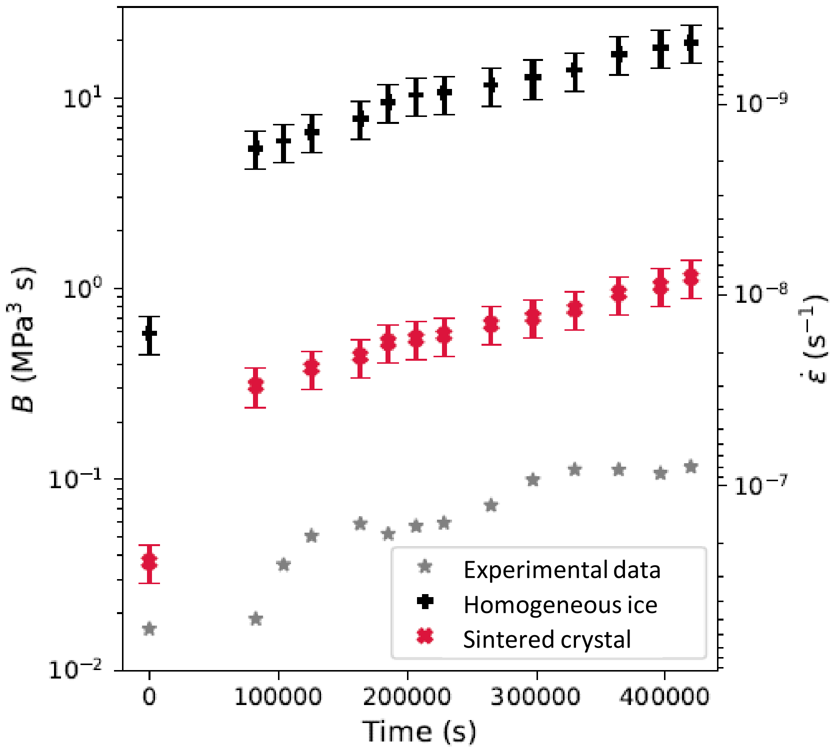
Homogeneous ice model

Sintered crystal model

- The gap between the two models decreases as density increases.



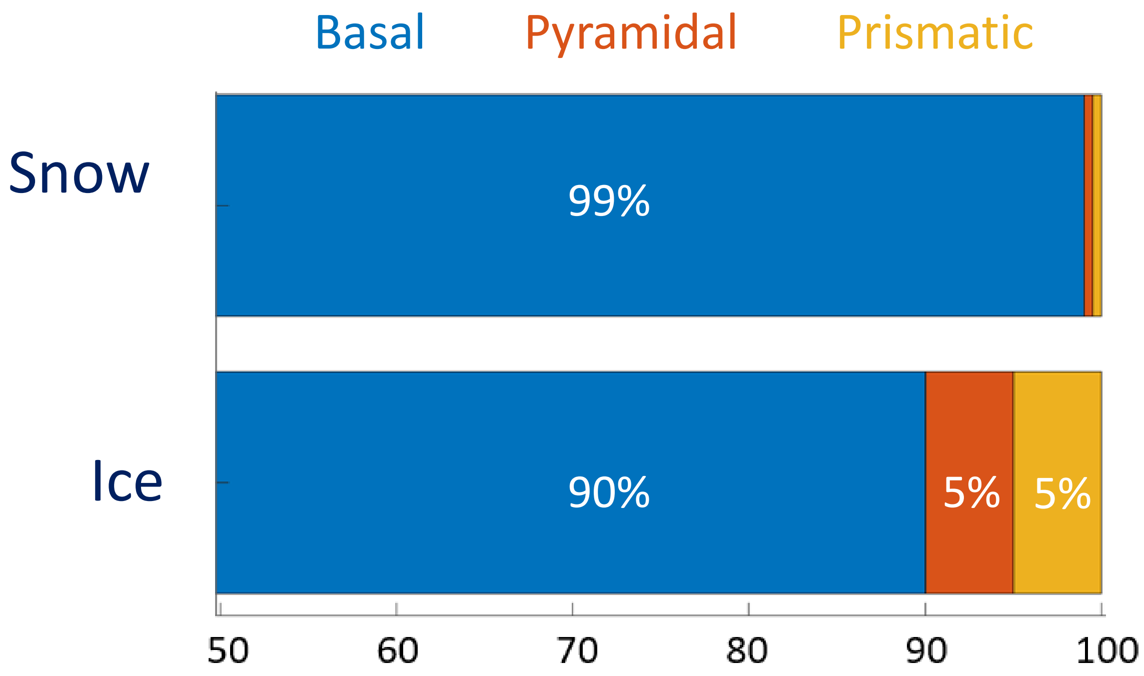
Strain-rate-controlled
$(\dot{\epsilon} = 1.8 \times 10^{-6}\ \mathrm{s}^{-1})$



Load-controlled
$(\sigma_{\mathrm{imp}} = 2.1\ \mathrm{kPa})$

Results: microscopic aspects of snow creep

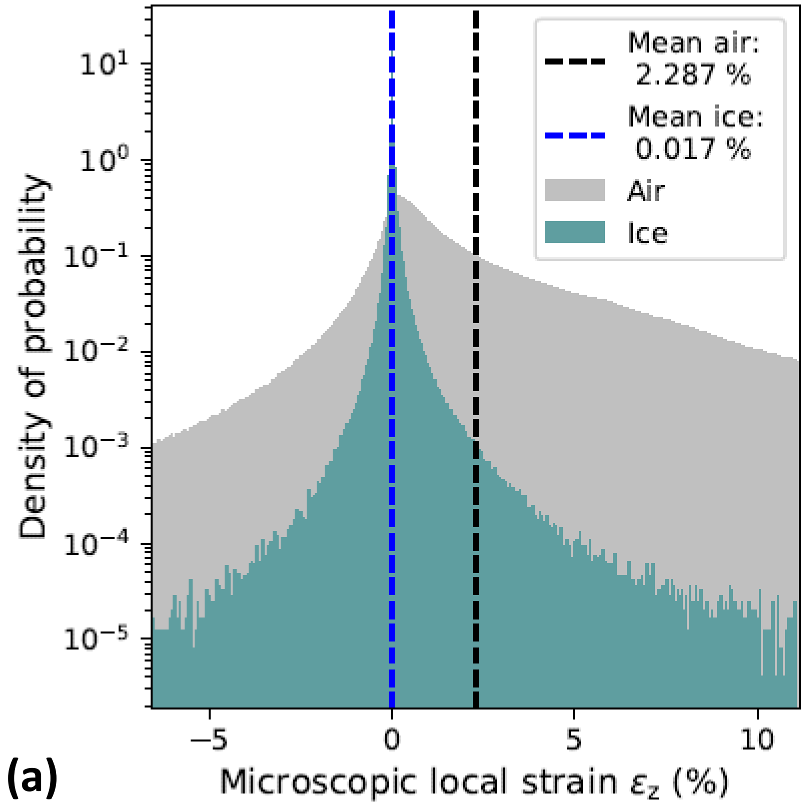
An accommodation of the basal slip different from ice!

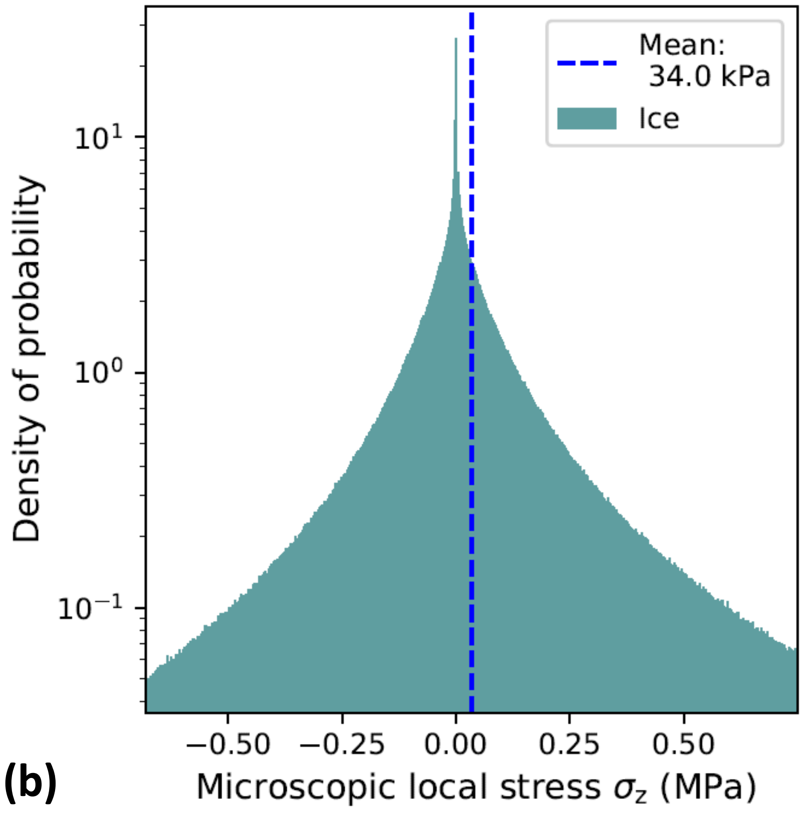


Contribution of the different glide systems on the microscopic equivalent slip $(\mathrm{p}_{\mathrm{eq}})$

- In snow : **accommodation** between crystals is permitted by the **pore space**

Results: microscopic aspects of snow creep

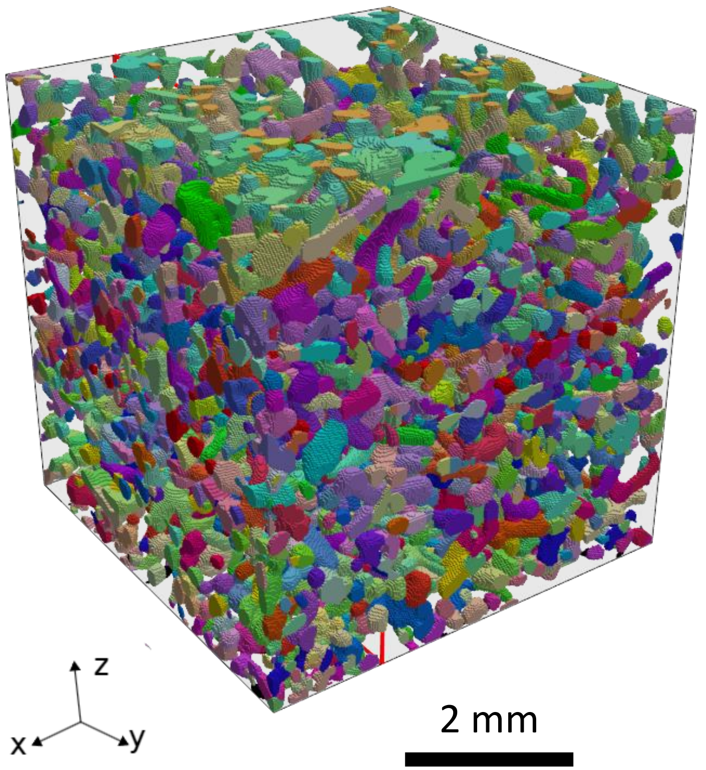




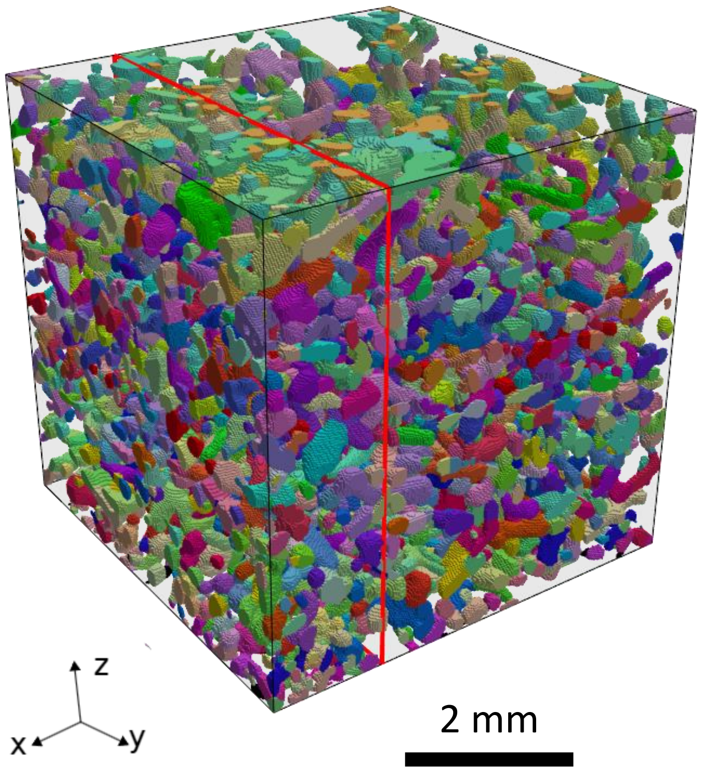
Histogram of the microscopic: (a) local strain ϵ_z distribution,
(b) vertical stress σ_z distribution.

- Macroscopic deformation is mainly due to **air deformation** and accommodation of the ice matrix.
- **Hight stress concentration:** 5 % of the microstructure reaches a vertical stress value higher than 0.51 MPa (58 times the macroscopic loading).

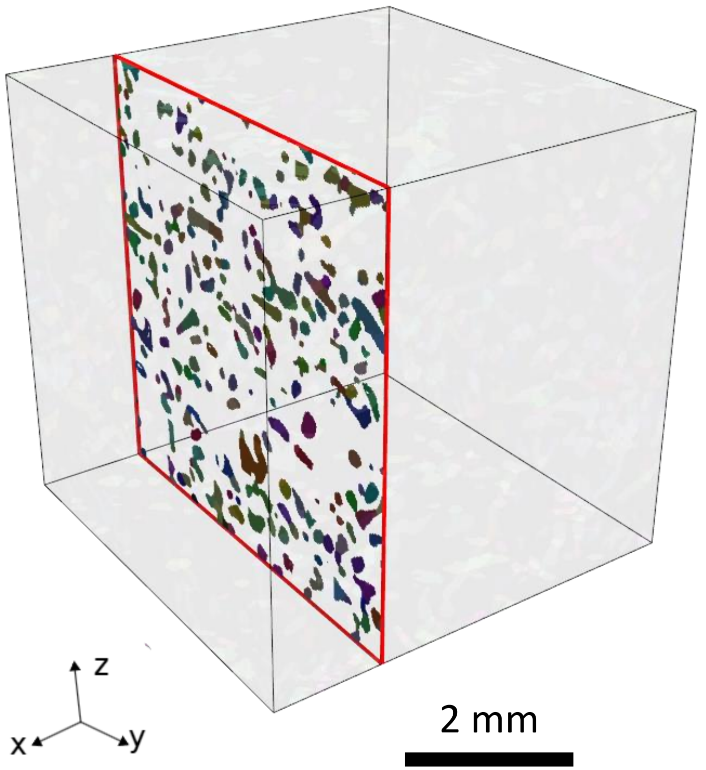
Results: microscopic aspects of snow creep



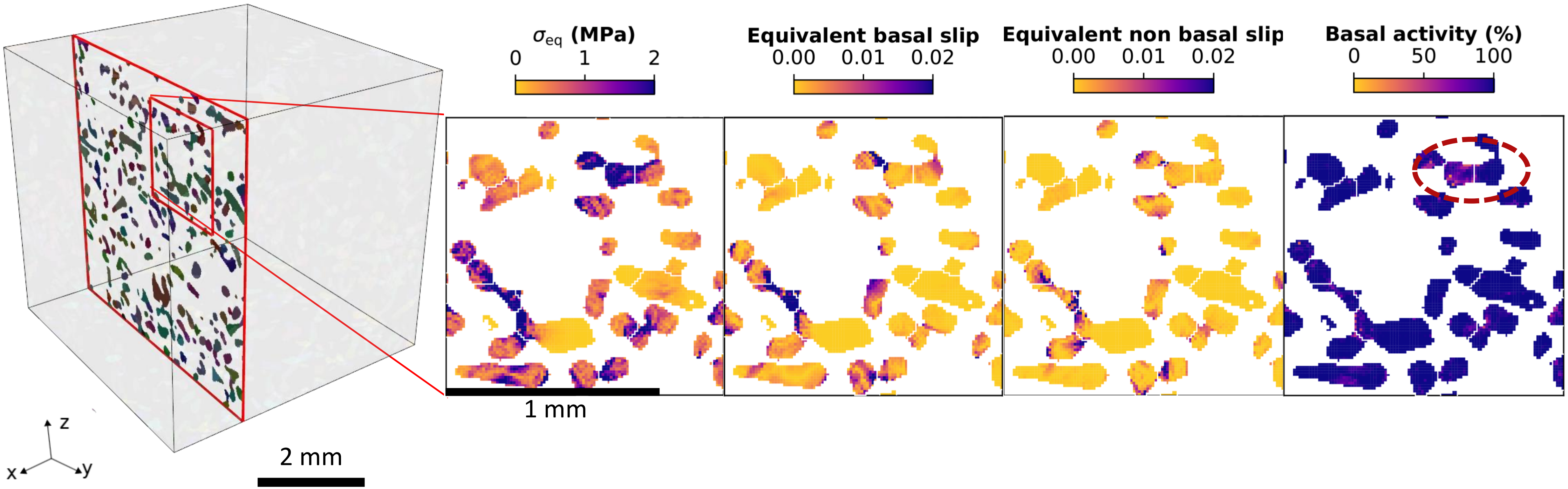
Results: microscopic aspects of snow creep



Results: microscopic aspects of snow creep



Results: microscopic aspects of snow creep

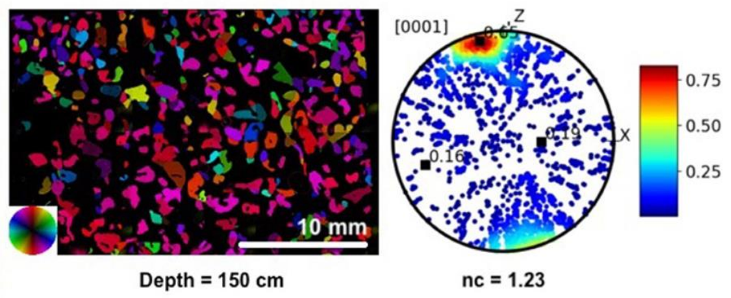


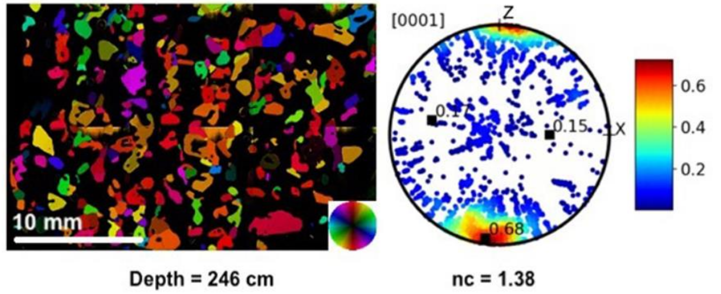
- ➢ Equivalent slip occurred preferentially at **crystal bond**, where stress is concentrated

Conclusion and outlooks

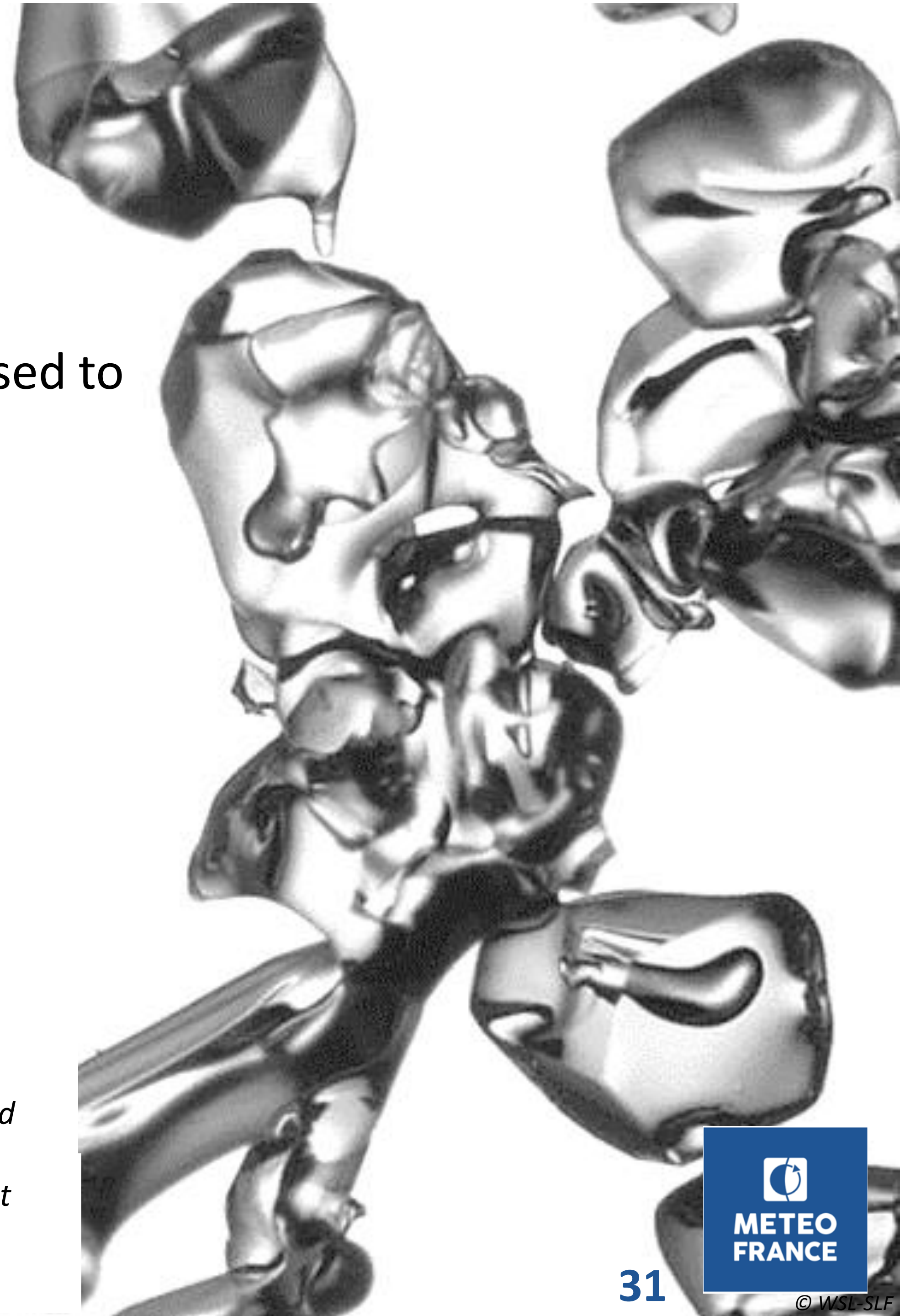
- First time that a **single-crystal plasticity model** has been used to study the mechanical behaviour of snow.

- Snow cannot be considered as a foam of ice, behaviour of **single-crystals** need to be considered.





Microstructure and C-axis pole figure from samples extracted at 150 (A) and 246 (B) cm depth along the EastGRIP snow pit (adapted from Montagnat et al., 2020)



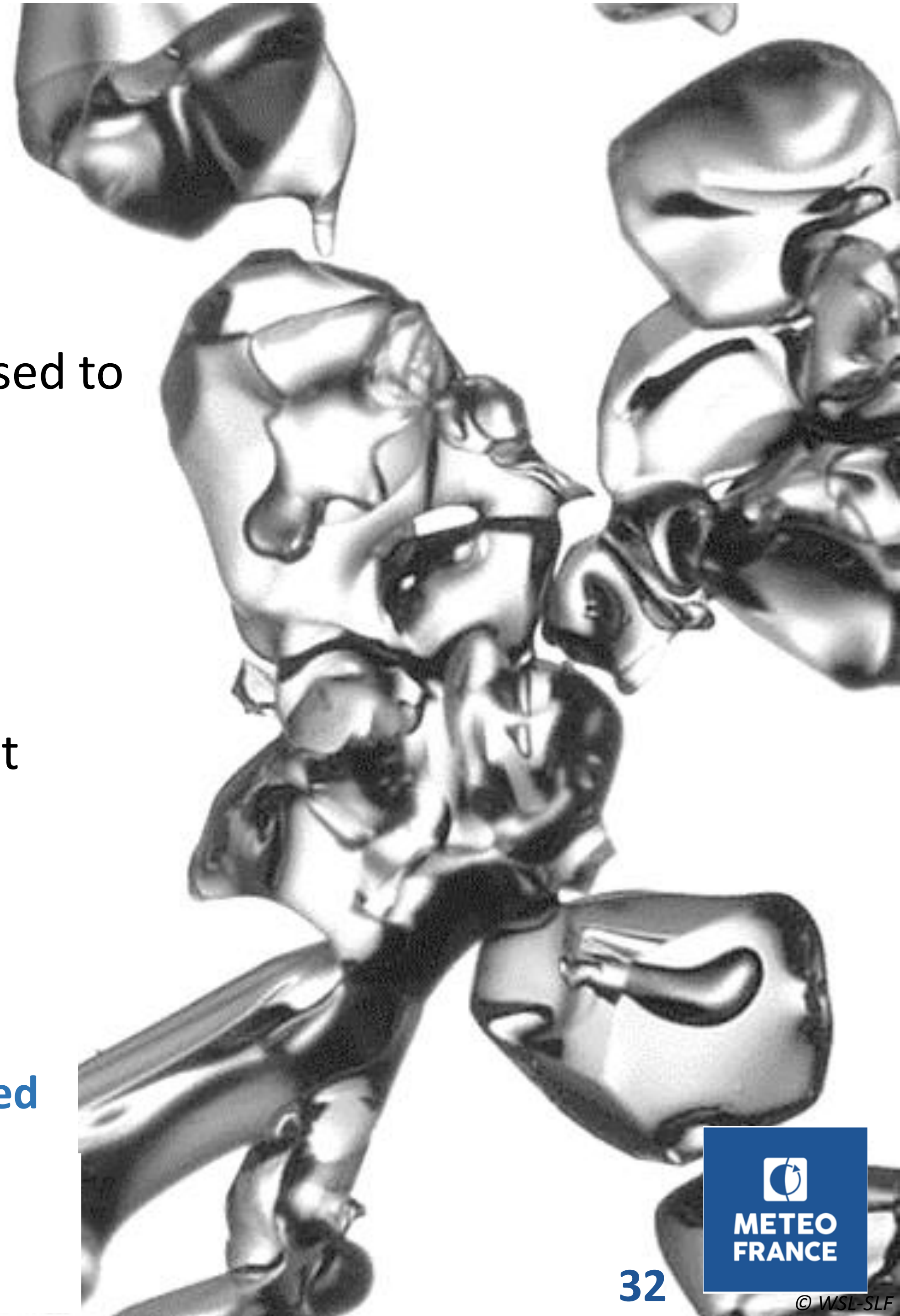
Conclusion and outlooks

➢ First time that a **single-crystal plasticity model** has been used to study the mechanical behaviour of snow.

➢ Snow cannot be considered as a foam of ice, behaviour of **single-crystals** need to be considered.

➢ Micro-scale mechanisms not yet understood, particularly at **grain boundaries**. Hypothesis:
  - ➢ Superplasticity (Alley, 1987, Raj & Ashby, 1971)
  - ➢ Ductile failure (Kirchner et al. 2001)

→ **New behaviour to model and further experiments planned**



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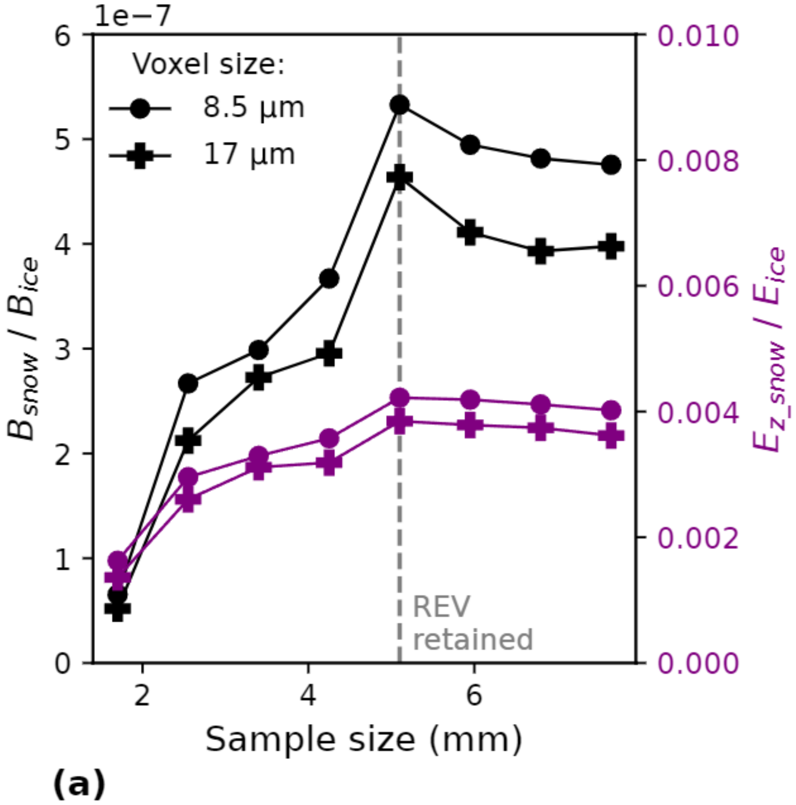
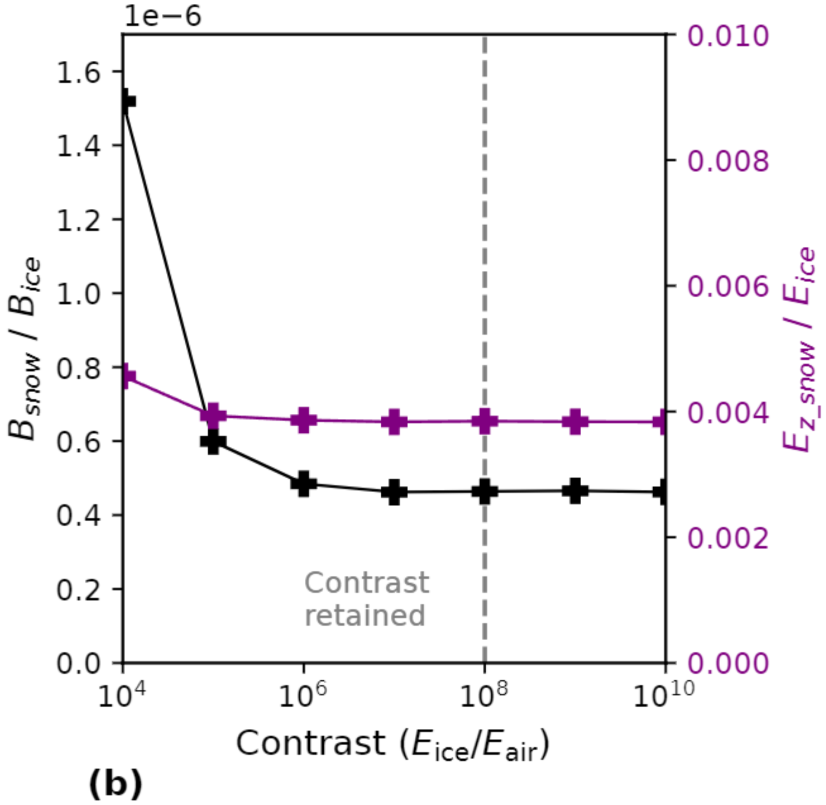
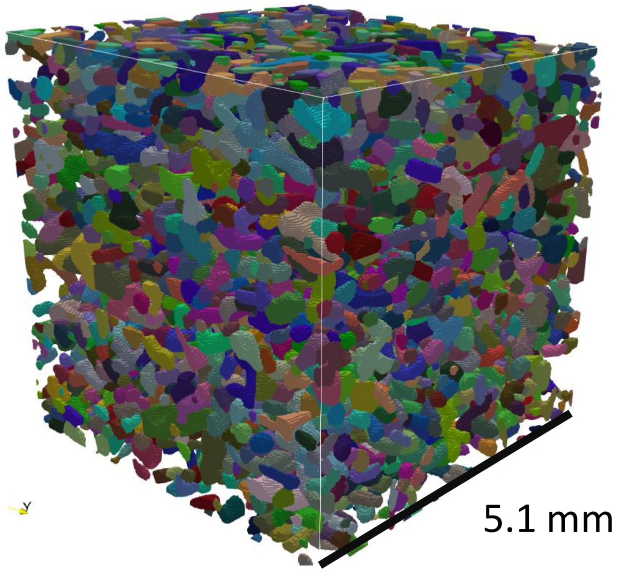
Appendix

Sensitivity analysis

Representative Elementary Volume and mechanical contrast







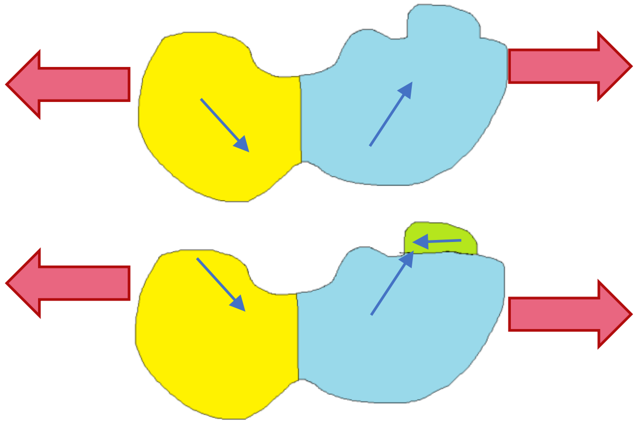
Sample studied.
Voxel size: 17 µm
$\rho = 255\ \mathrm{kg\ m^{-3}}, r_{\mathrm{eq}} = 121\ \mu\mathrm{m},$

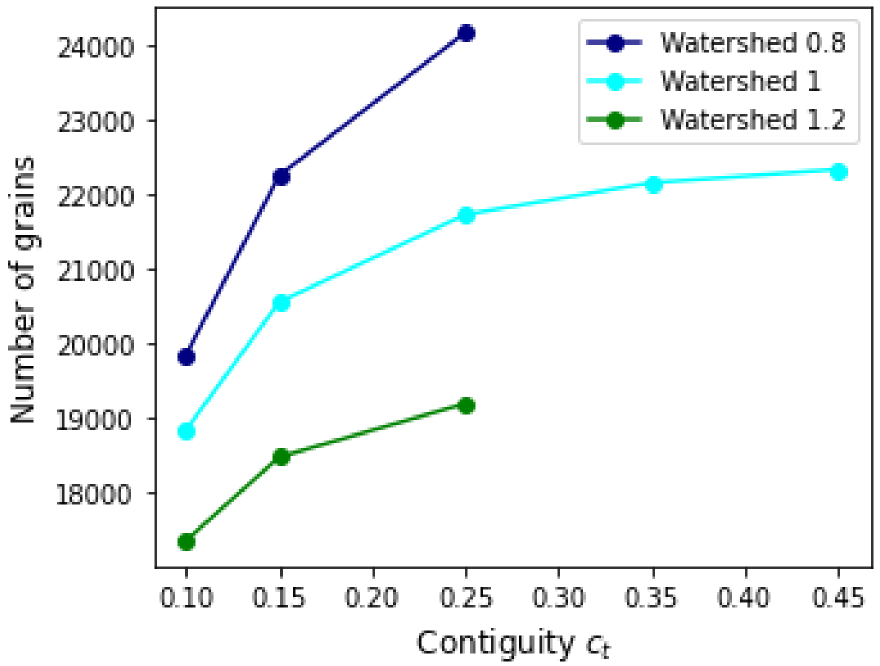
Convergence analysis of the nonlinear viscosity and Young's modulus with respect to: ***(a)*** *the sample length and* ***(b)*** *the mechanical contrast.*

Sensitivity analysis

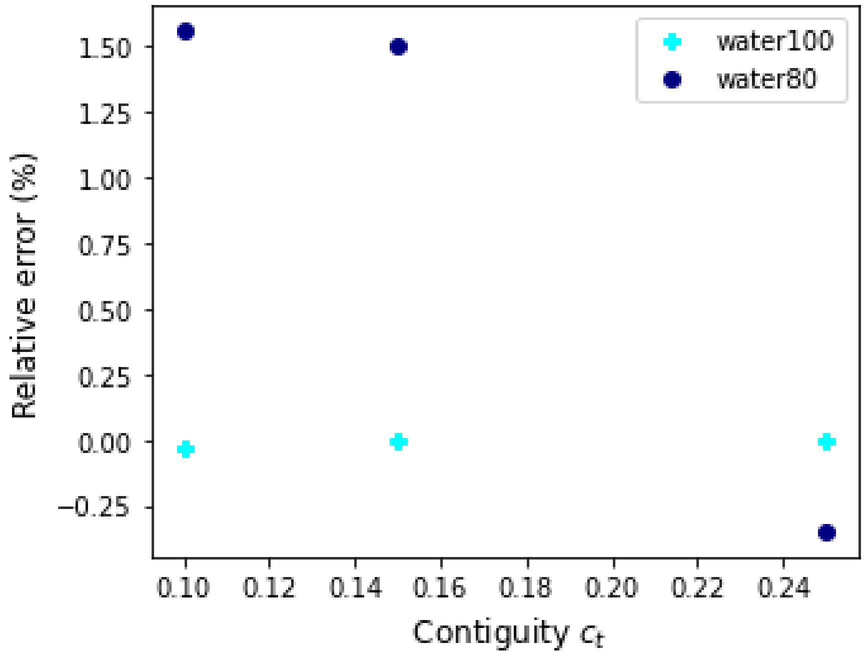
Grain segmentation

Low effect compared to uncertainty (REV, temperature, experimental measurement)



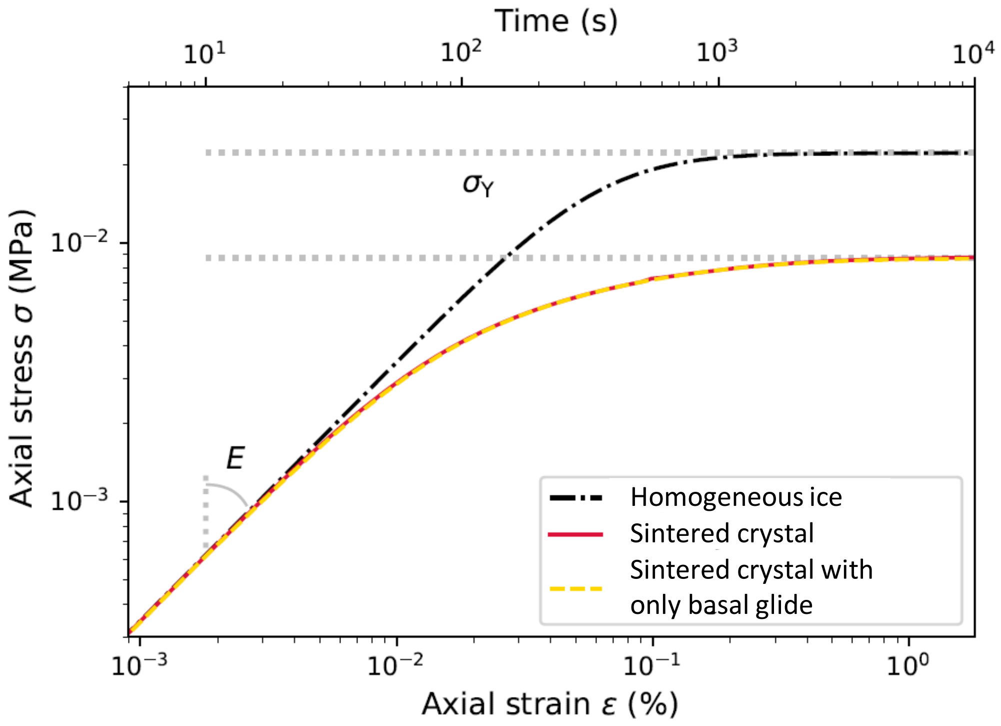


Number of geometrical grains as a function of c_t for different values of $\tilde{\kappa}_t$.

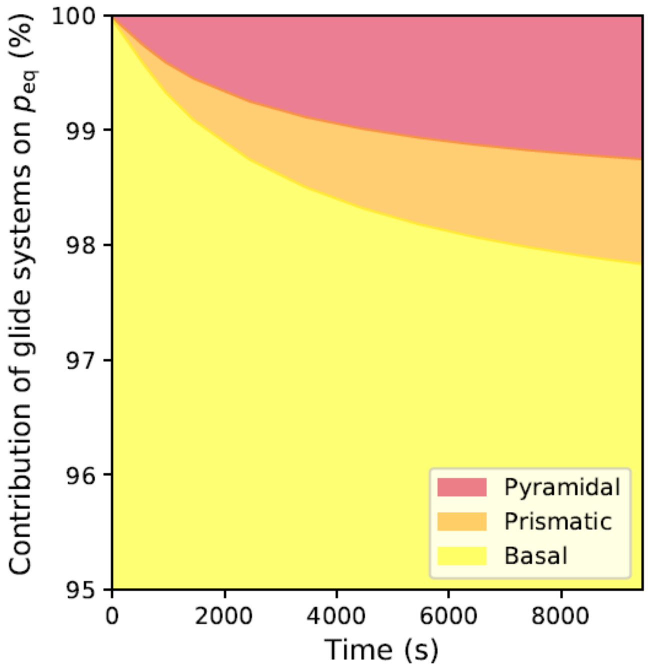


Relative error in the calculation of the snow B as a function of c_t for different values of $\tilde{\kappa}_t$ (reference $c_t = 0.15$; $\tilde{\kappa}_t = 1$)

Influence of non-basal slip systems:

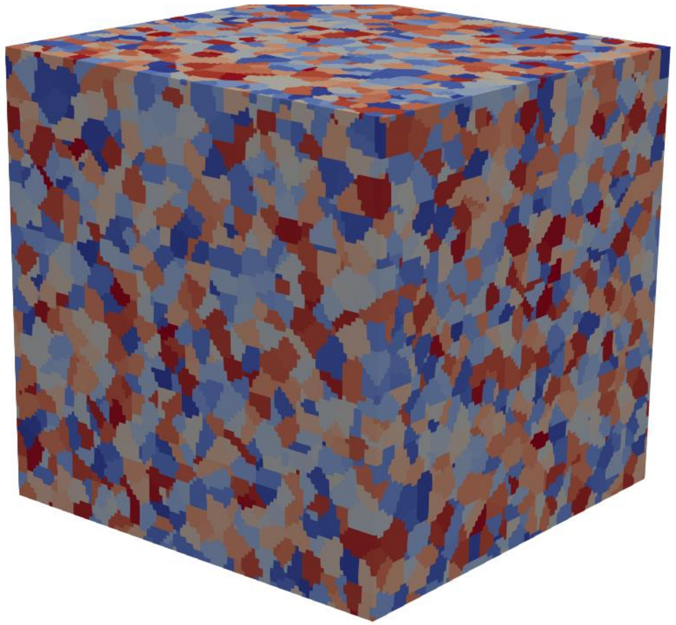


Evolution of yield stress with the strain for the different constitutive equations of ice.



Temporal evolution of the contribution of the different glide systems on the microscopic equivalent slip $(\mathrm{p_{eq}})$

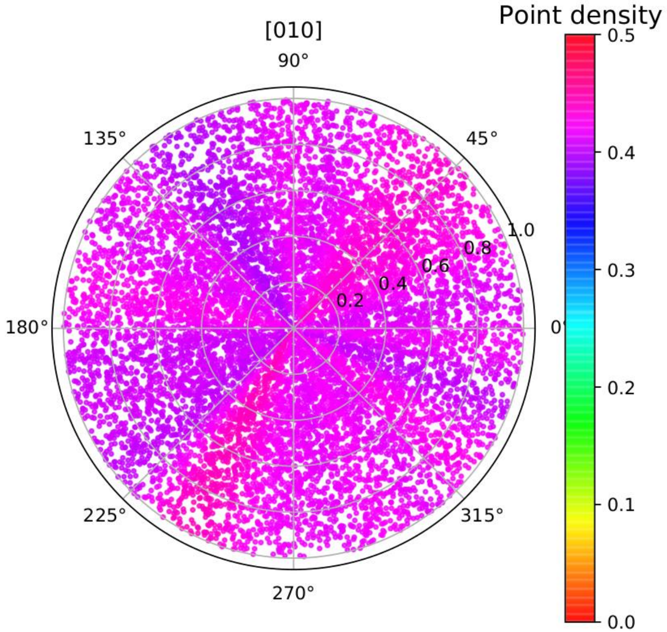
Preliminary study:
Modelling of the viscoplastic behaviour of ice



Voronoi, 9261 grains, 106^3 voxels

Implementation of the two material laws:

- polycrystalline
- monocrystalline: unknown grain orientation, random draw c-axis



Pole figure, plan (X,Z)

Boundary conditions:
Constant strain rate compression test with stress-free boundary condition

Elasto-viscoplasticity: preliminary study
Modelling of the viscoplastic behaviour of ice

Macroscopic laws identified:

- Polycristalline model:

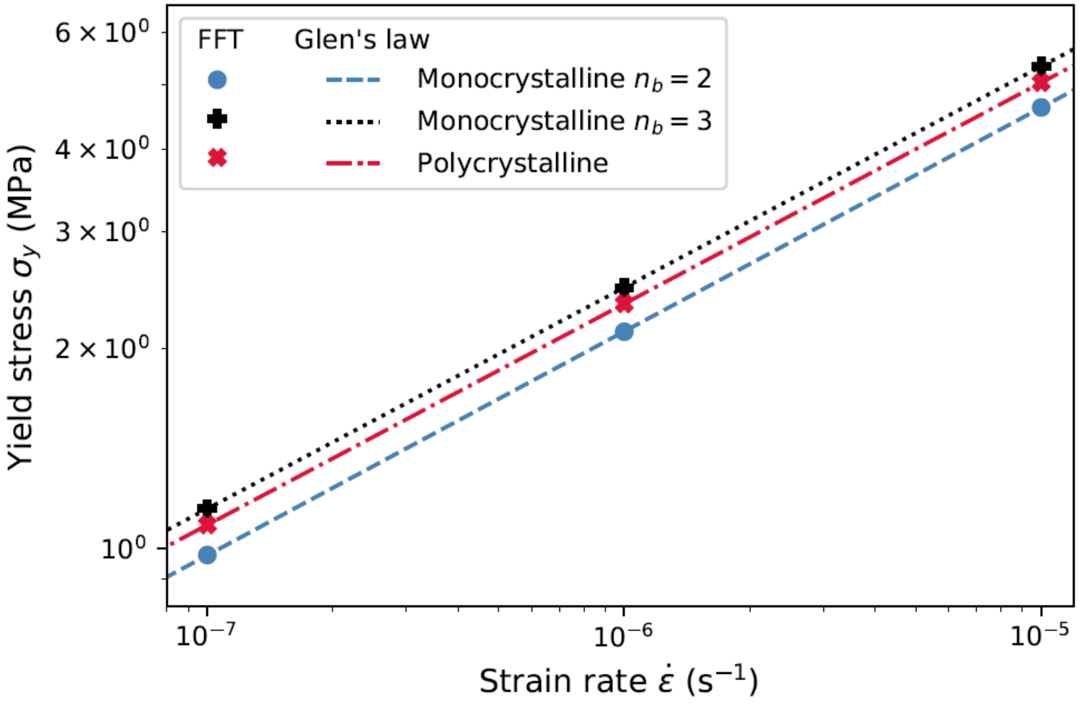
$$\dot{\epsilon} = 7.8 \times 10^{-8}\ \sigma_Y^3$$

- Monocristalline model ($n_{basal} = 3$):

$$\dot{\epsilon} = 6.59 \times 10^{-8}\ \sigma_Y^3$$

- Macroscopic laws identified ($n_{basal} = 2$):

$$\dot{\epsilon} = 1.12 \times 10^{-8}\ \sigma_Y^{2.96}$$

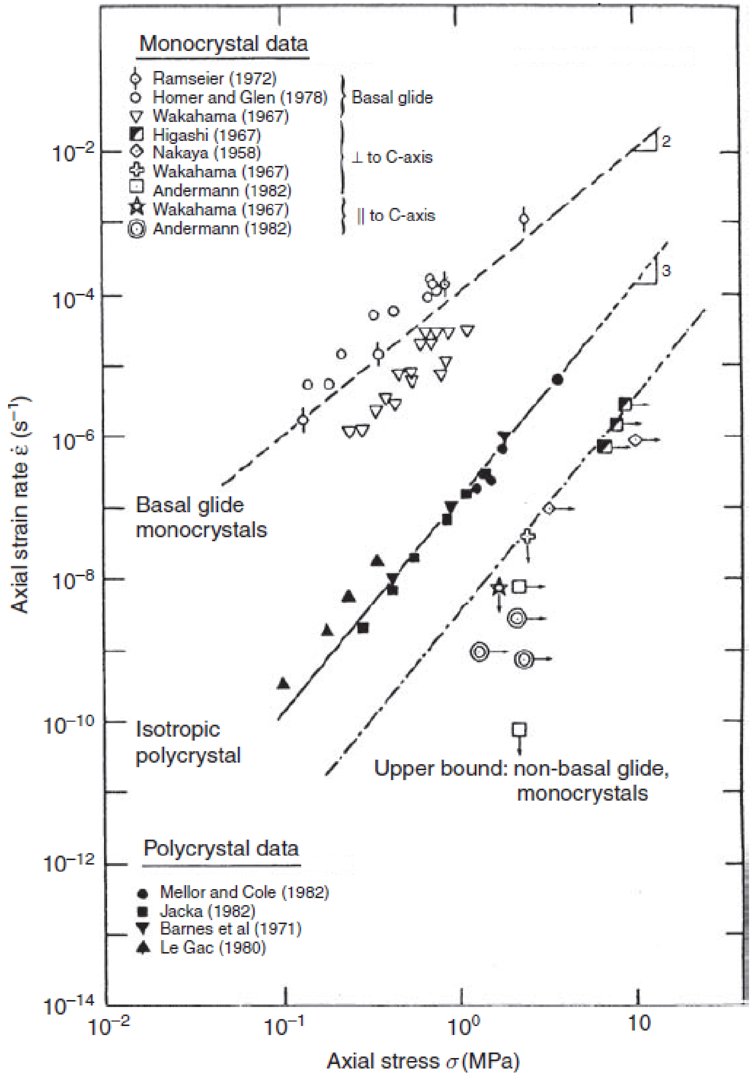


- Simplified geometry
- Incertainties on the prefactor A of $\pm 25\%$
  - ➢ Neglieable compared to error commited on snow

Limits and outlooks

- Basal slip system is main deformation mechanism
- Experiments show that basal slip system has an exponent **2** (3 for all systems in our study)
  - need to **calibrate a new crystal plasticity** model on polycrystalline ice

- **Homogenization of an elasto-viscoplastic law** for a wide range of snow microstructures, to develop improved formulations of snow settlement in detailed snowpack simulation tools.



Stress–strain rate relationship for steady-state basal and non-basal slip in single crystals at −10 °C. (Schulson and Duval, 2009)