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PART II: The legacy of isotropic ice

1. A flow law for ice: experimental evidence

2. A flow law for ice: continuum mechanical modeling

3. Microscale processes beyond secondary creep

1. A flow law for ice: experimental evidence

Experimental in-situ validation
of any flow law for ice is difficult:

- extremely long time scales
- Flow-Structure-**E**nvironment-**I**nterplay

Experimental validation in the lab
suffers from

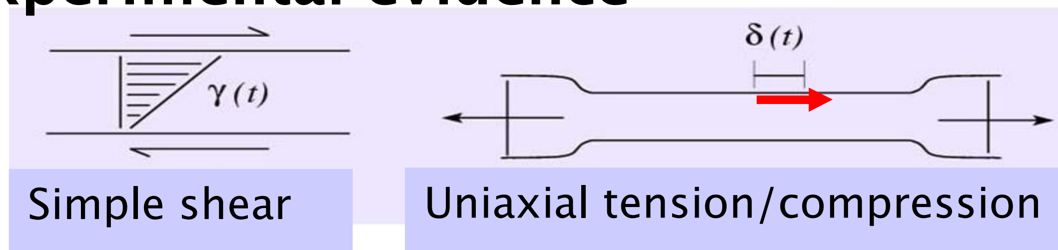
- limitations in test-duration
- constrained dimensions
- limited/no account of FSEI

BUT:
analogies to high temperature alloys/
metal crystal plasticity (since early 20th
century, von Mises etc.)

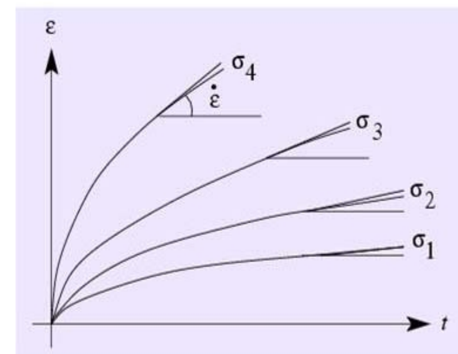
1. A flow law for ice: experimental evidence

Ice in the lab: since ~1950

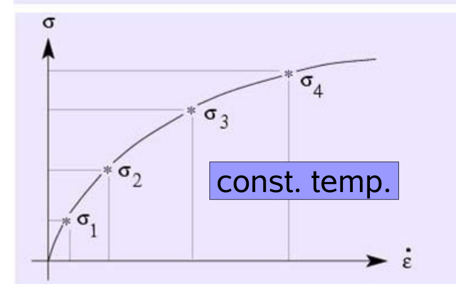
- Early experiments:



Simple shear, uniaxial tension/compression at constant force (stress) or constant strain rate and prescribed temperature

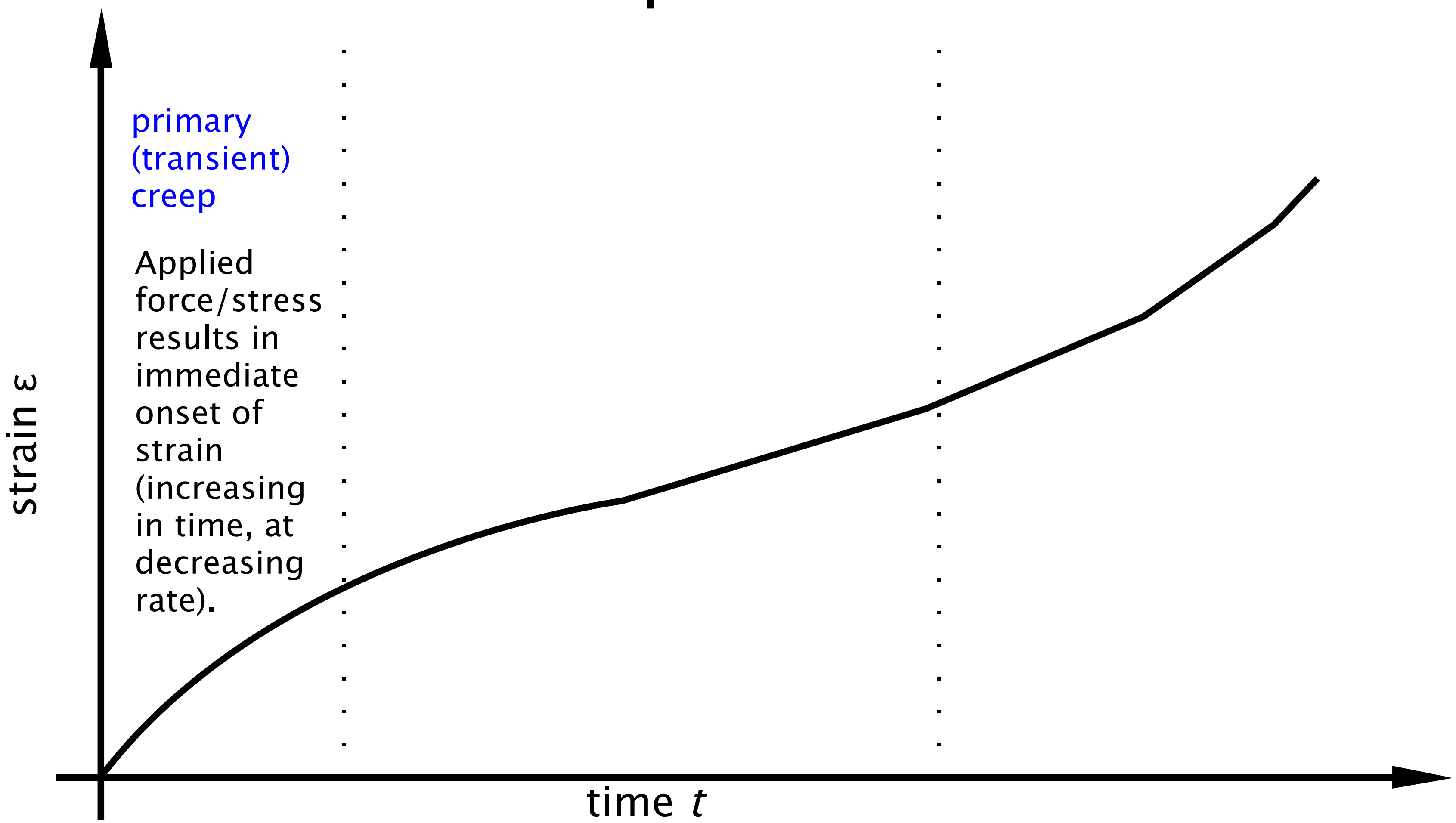


- For constant stress experiments
  - Applied force is monitored
  - Deformation $\gamma(t)$, $\delta(t)$ is measured



- For constant strain rate experiments
  - Certain components of deformation are monitored
  - Forces are measured

1. A flow law for ice: experimental evidence



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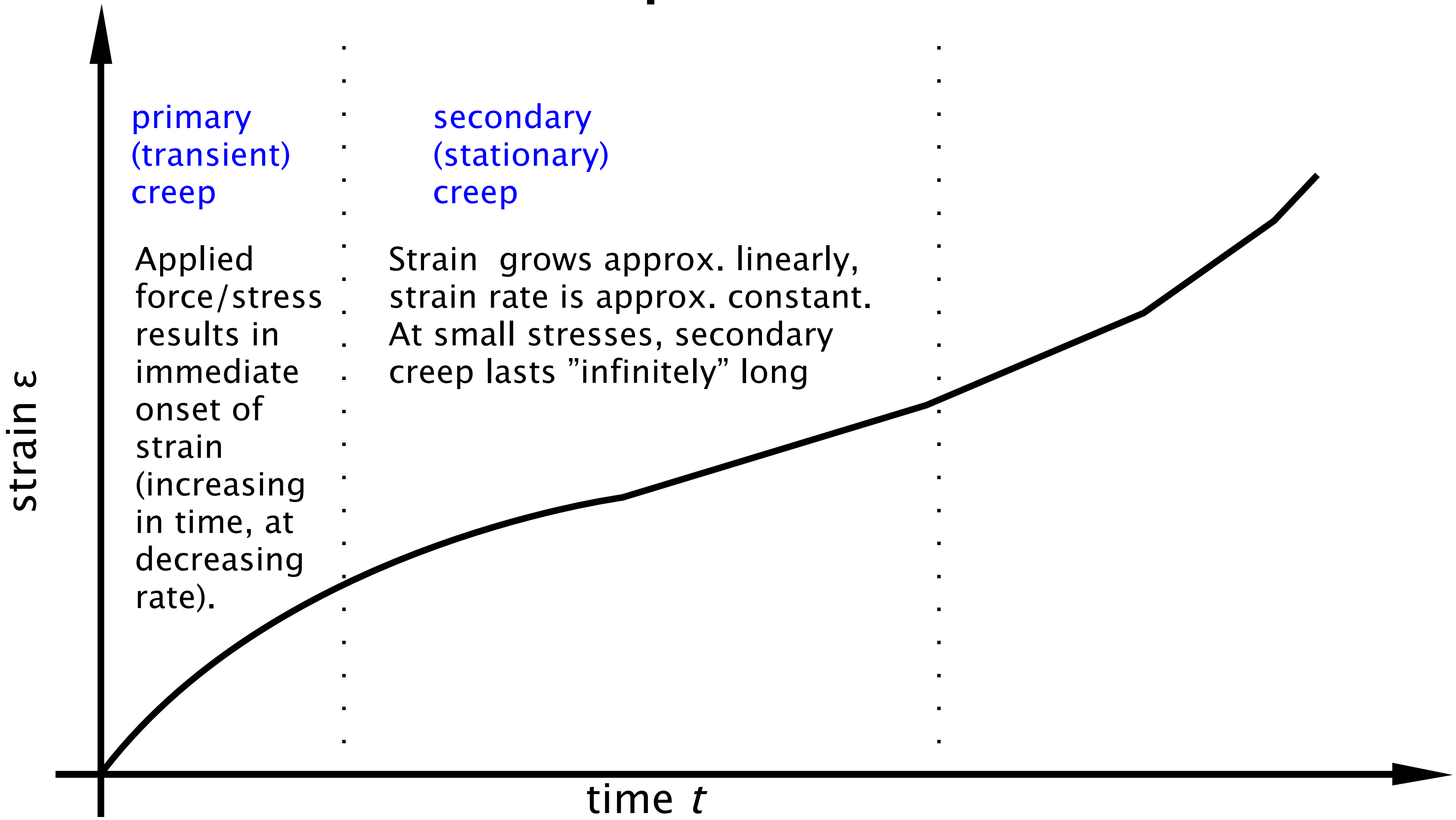

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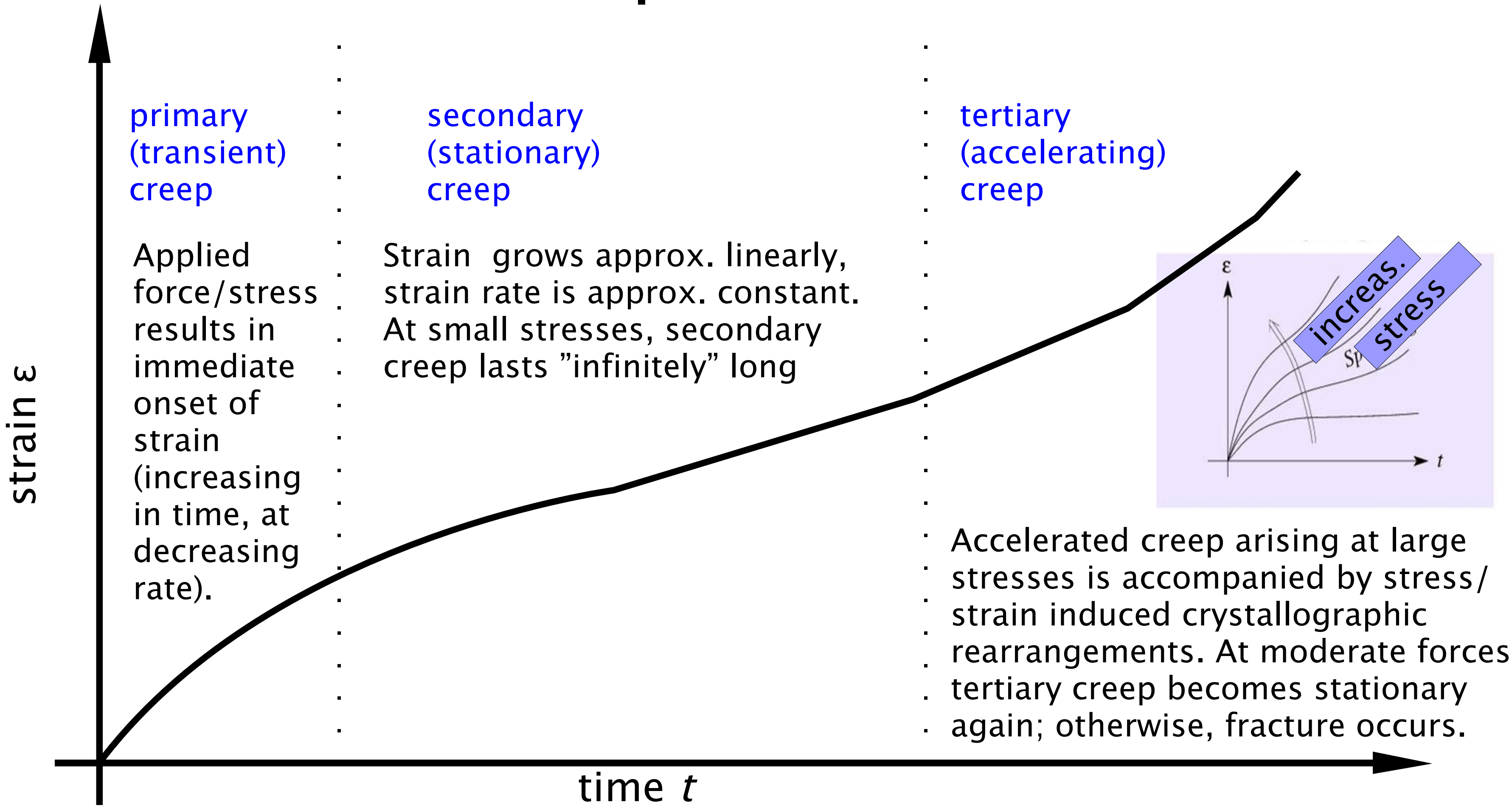
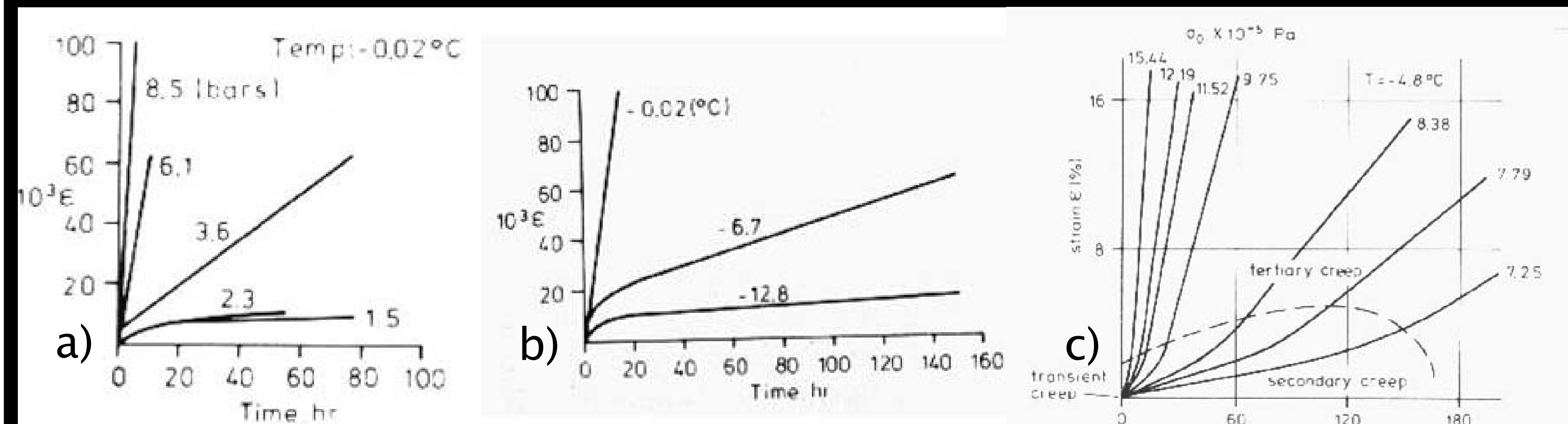


1. A flow law for ice: experimental evidence

Measured creep curves

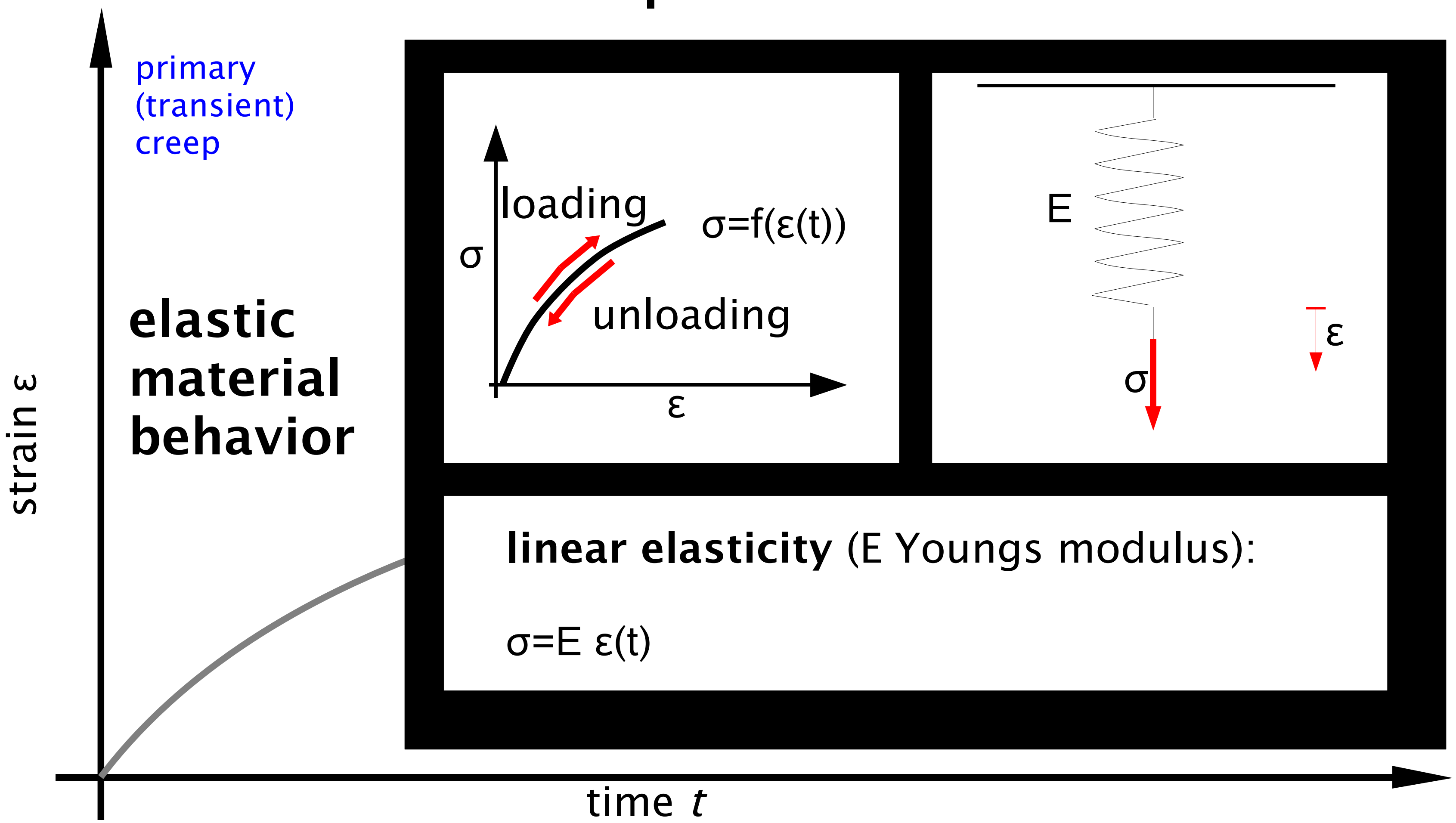


a) Creep curves for isotropic polycrystalline ice at stresses between 0.15 MPa and 0.85 MP (Glen, 1953)

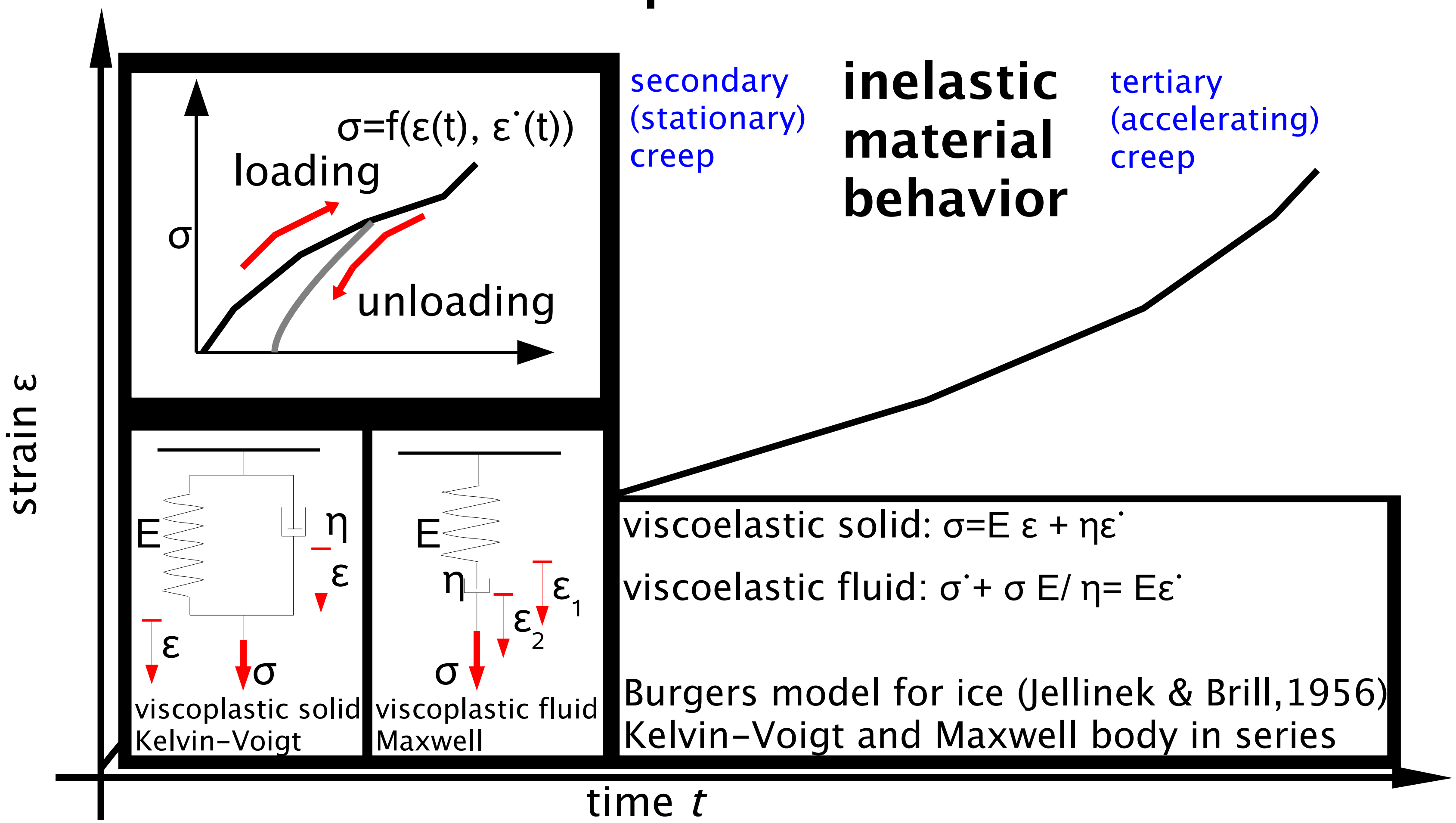
b) Creep curves for isotropic polycrystalline ice at various temperatures and a pressure of 0.6 MPa (Glen, 1953)

c) Creep curves for isotropic polycrystalline ice at -4.8 deg C at stresses between 0.7 MPa and 1.54 MPa (Steinemann, 1958)

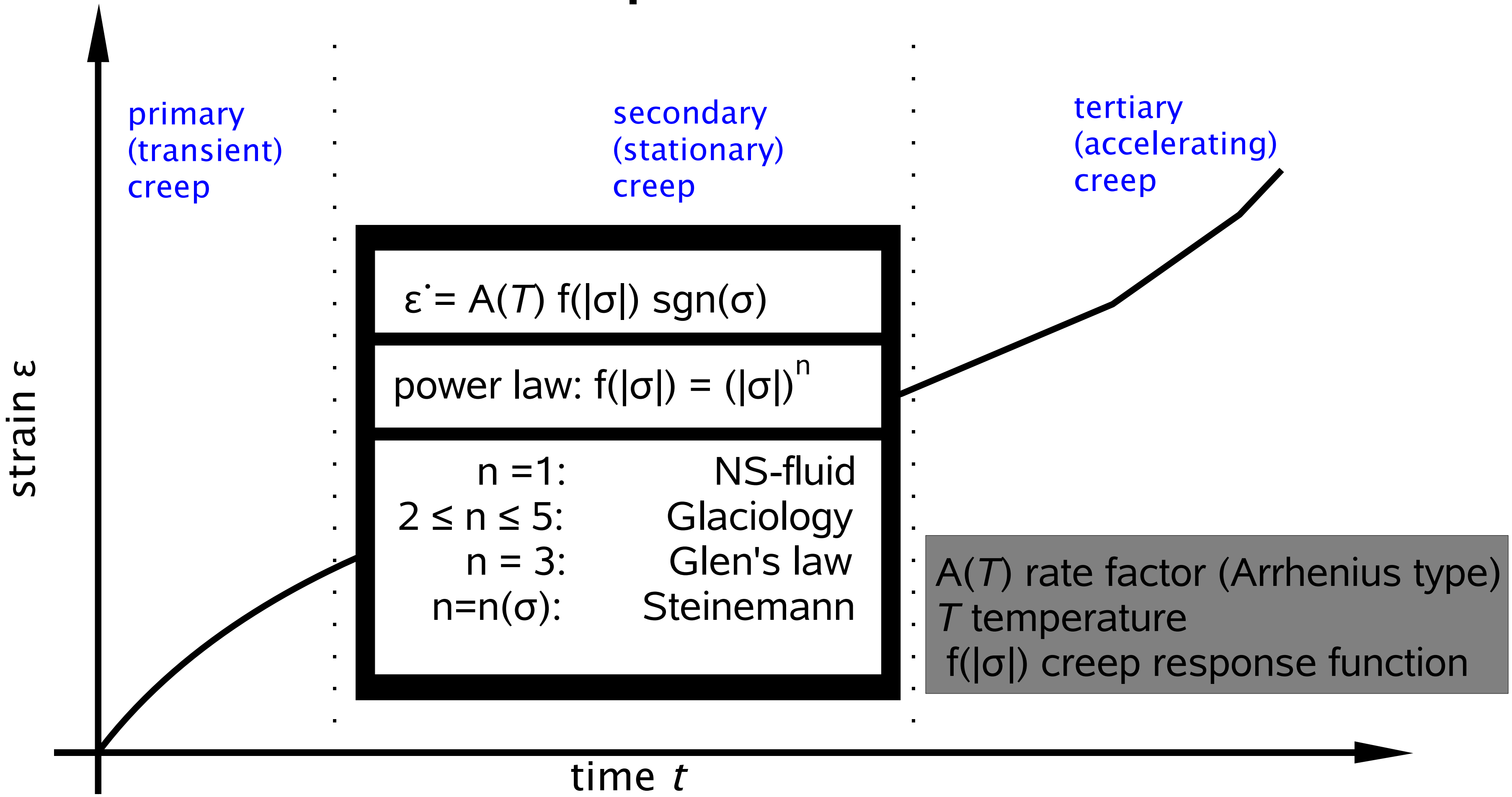
1. A flow law for ice: experimental evidence



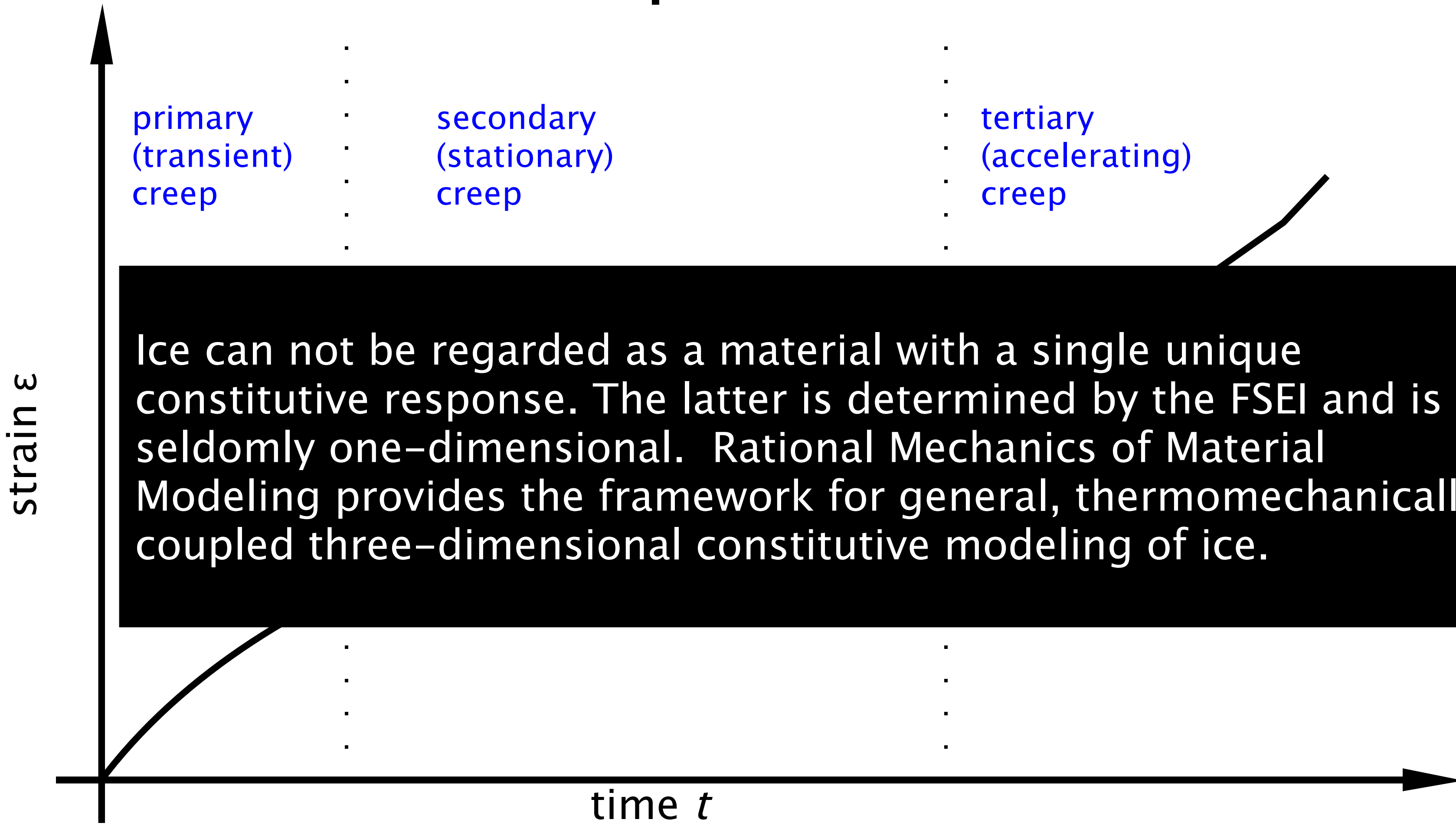
1. A flow law for ice: experimental evidence



1. A flow law for ice: experimental evidence



1. A flow law for ice: experimental evidence



Ice can not be regarded as a material with a single unique constitutive response. The latter is determined by the FSEI and is seldomly one-dimensional. Rational Mechanics of Material Modeling provides the framework for general, thermomechanically coupled three-dimensional constitutive modeling of ice.

2. A flow law for ice: continuum mechanical modeling

The behavior of any material body on Earth is such that it obeys

- conservation of mass
- conservation of linear momentum
- conservation of energy

$$\dot{\rho} + \rho \mathrm{div}\mathbf{v} = 0$$
$$\rho\dot{\mathbf{v}} = \mathrm{div}\,\mathbf{T} + \rho\mathbf{g}$$
$$\rho\dot{\varepsilon} = -\mathrm{div}\mathbf{q} + \mathrm{tr}(\mathbf{D}\cdot\mathbf{T}) + \rho r$$

Material specific behavior enters through

- restrictions on the spatio-temporal variation of the fields involved (e.g. incompressibility, represented by $\dot{\rho}=0$)
- prescription of constitutive relations (e.g. a ”flow-law” for the stress)

2. A flow law for ice: continuum mechanical modeling

Constitutive equations

- relate heat flux **q** and internal energy ε to temperature *T*

$$\mathbf{q} = -\kappa(T)\,\mathrm{grad}\,T$$

$$\dot{\varepsilon}(T) = c_p(T)\dot{T}$$

- relate stress **T** to e.g. velocity **v** and temperature *T*

$$\mathbf{T} = \hat{\mathbf{T}}(\rho, \mathbf{v}, T)$$

$$\mathbf{T}^E = \hat{\mathbf{T}}^E(\mathbf{D} = \mathrm{sym\,grad}\,\mathbf{v}, T)$$

"Inversion"

$$\mathbf{D} = \hat{\mathbf{D}}(\mathbf{T}^E, T)$$

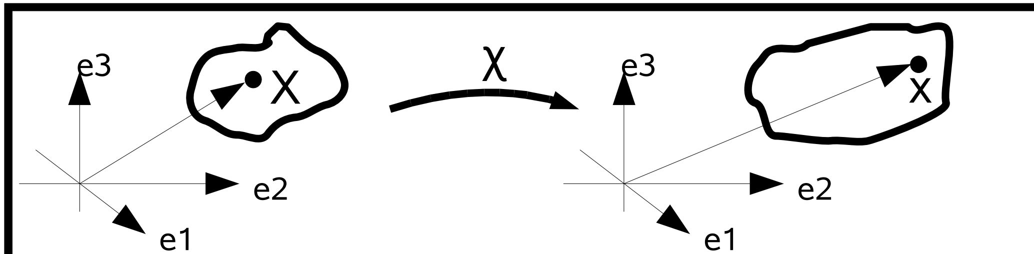
$$\mathbf{v} = (v_x(x,y,z,t), v_y(x,y,z,t), v_z(x,y,z,t))$$

$$\mathbf{T} = -p\mathbf{I} + \mathbf{T}^E = -p\mathbf{I} + \begin{pmatrix} \tau_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{xy} & \tau_{yy} & \tau_{yz} \\ \tau_{xz} & \tau_{yz} & \tau_{zz} \end{pmatrix}$$

2. A flow law for ice: continuum mechanical modeling

Generalizing $\dot{\varepsilon} = A(T)\, f(|\sigma|)\, \mathrm{sgn}(\sigma)$ (Glen–Steinemann) to a 3-d law ?

Material Modeling: the ”Rational Mechancis” approach
(C. Truesdell, R.A. Toupin, W. Noll, 1960ies, Hutter & Jöhnk, 2004)



χ motion function
X,x position of particle in reference/present configuration

2. A flow law for ice: continuum mechanical modeling

Generalizing $\dot{\varepsilon} = A(T)\, f(|\sigma|)\, \mathrm{sgn}(\sigma)$ (Glen–Steinemann) to a 3-d law ?

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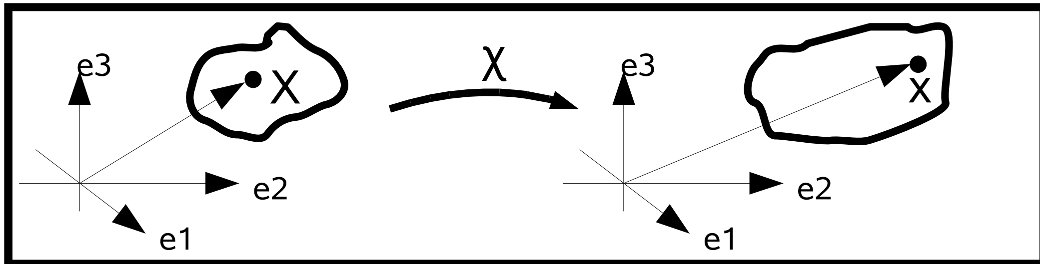


χ	motion function
X,x	position of particle in reference/present configuration

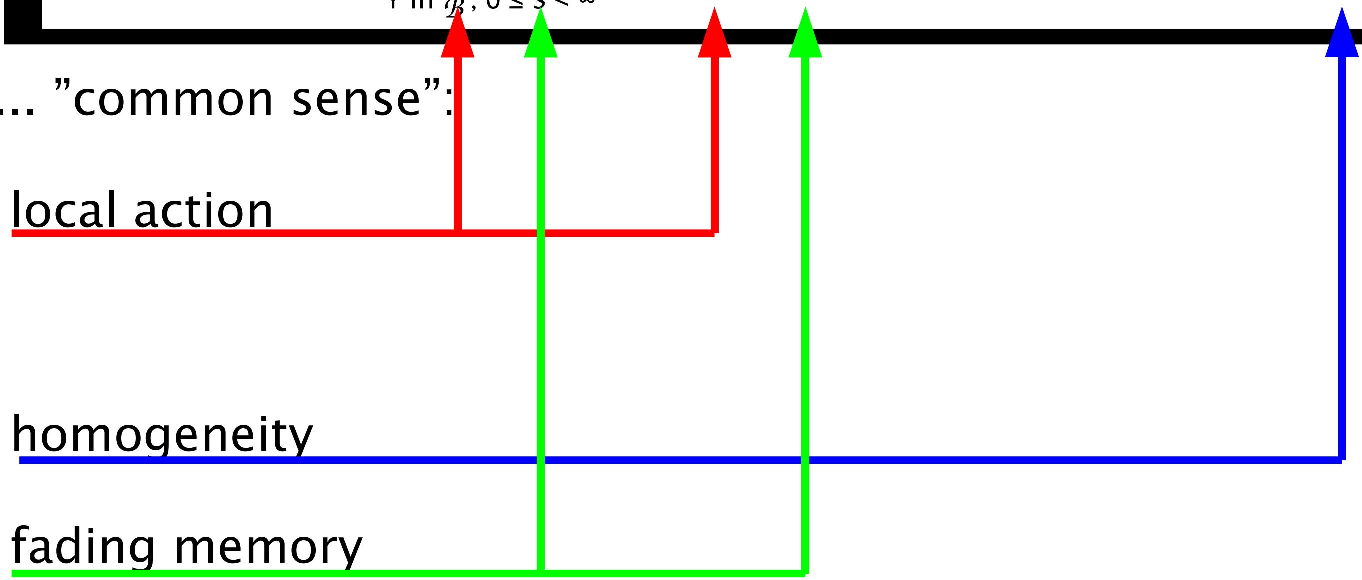
- define a set S of independent, primary variables: $S=\{\rho, T, \mathbf{v}, \ldots\}$
- define a set C of dependent, constitutive quantities: $C = \{\mathbf{T}, \mathbf{q}, \varepsilon, \ldots\}$
- constitutive relation: $\mathbf{T}(X, t) = \check{\mathbf{T}}_{Y \text{ in } \mathcal{B},\, 0 \le s < \infty}\left(\chi(Y, t-s), \rho(Y, t-s), T(Y, t-s), X\right)$

respects: determinism, inhomogeneity, non-local effects, rule of equipresence

2. A flow law for ice: continuum mechanical modeling

Simplification of general constitutive relations achieved by application of ...

$$\mathbf{T}(X,\, t) = \check{\mathbf{T}}_{Y \text{ in } \mathcal{B},\, 0 \leq s < \infty} \left(\chi(Y,\, t-s),\, \rho(Y,\, t-s),\, T(Y,\, t-s),\, X \right)$$



.... ”common sense”:

- local action
- homogeneity
- fading memory

2. A flow law for ice: continuum mechanical modeling

Simplification of general constitutive relations achieved by application of ...

$$\mathrm{T}(X,\ t) = \check{\mathrm{T}}_{Y\ \mathrm{in}\ \mathcal{B},\ 0 \le s < \infty}\left(\chi(Y,\ t-s),\ \rho(Y,\ t-s),\ T(Y,\ t-s),\ X\right)$$

.... ”common sense”:

- local action
- homogeneity
- fading memory

... Rational Mechanics principles:

- **invariance under change of observer** and **rule of material indifference** (**principle of objectivity**)
- **principle of material symmetry**
- **entropy principle** (2nd law of thermodynamics)

2. A flow law for ice: continuum mechanical modeling

Example: the stress tensor for a linear elastic solid

functional dependence: $\mathbf{T}=\check{\mathbf{T}}(\mathbf{F})$ $\mathbf{F}=F_{iA}=\partial x_i / \partial X_A$

2. A flow law for ice: continuum mechanical modeling

Example: the stress tensor for a linear elastic solid

functional dependence: $\mathbf{T} = \check{\mathbf{T}}(\mathbf{F})$ $\mathbf{F} = F_{iA} = \partial x_i / \partial X_A$

material objectivity: $\mathbf{T} = \check{\mathbf{T}}(\mathbf{F}) = \check{\mathbf{T}}(\mathbf{E})$ $2\mathbf{E} = (\mathbf{F}^T\mathbf{F} - \mathbf{1})$

Green–Lagrange strain tensor

2. A flow law for ice: continuum mechanical modeling

Example: the stress tensor for a linear elastic solid

functional dependence:	$\mathbf{T}=\check{\mathbf{T}}(\mathbf{F})$	$\mathbf{F}=F_{iA}= \partial x_i / \partial X_A$
material objectivity:	$\mathbf{T}=\check{\mathbf{T}}(\mathbf{F}) = \check{\mathbf{T}}(\mathbf{E})$	$2\mathbf{E}= (\mathbf{F}^T\mathbf{F}-\mathbf{1})$ Green-Lagrange strain tensor
entropy principle:	$\mathbf{S} = \rho\, \partial\Psi / \partial \mathbf{E}$	Ψ Helmholtz energy **S** Piola-Kirchhoff stress tensor

2. A flow law for ice: continuum mechanical modeling

Example: the stress tensor for a linear elastic solid

functional dependence:	$\mathbf{T}=\check{\mathbf{T}}(\mathbf{F})$	$\mathbf{F}=F_{iA}= \partial x_i / \partial X_A$
material objectivity:	$\mathbf{T}=\check{\mathbf{T}}(\mathbf{F}) = \check{\mathbf{T}}(\mathbf{E})$	$2\mathbf{E}= (\mathbf{F}^T\mathbf{F}-\mathbf{1})$ Green-Lagrange strain tensor
entropy principle:	$\mathbf{S} = \rho\, \partial\Psi / \partial \mathbf{E}$	Ψ Helmholtz energy $\mathbf{S}$ Piola-Kirchhoff stress tensor
linear behavior:	$2\Psi=\mathbf{E}\,(\mathbf{C}^{(4)}\,\mathbf{E})$	Ψ: quadratic in $\mathbf{E}$ $\mathbf{C}^{(4)}$: elasticity tensor with 81 components

2. A flow law for ice: continuum mechanical modeling

Example: the stress tensor for a linear elastic solid (ctnd)

symmetry properties of $\mathbf{C}^{(4)}$ (81 independent components):

S and **E** are symmetric tensors: $\mathbf{C}^{(4)}$ has 36 independent components

S derivable from the potential Ψ: $\mathbf{C}^{(4)}$ has 21 independent components

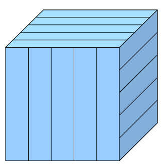
Voigt notation: $\boldsymbol{\Sigma} = \mathbf{C}^{*(2)}\,\boldsymbol{\Xi}$

$\boldsymbol{\Sigma} = (S_{11}, S_{22}, S_{33}, S_{12}, S_{13}, S_{23})$, $\boldsymbol{\Xi} = (E_{11}, E_{22}, E_{33}, E_{12}, E_{13}, E_{23})$

$C^{*(2)}$ symmetric 6 x 6 matrix

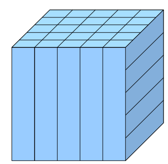
2. A flow law for ice: continuum mechanical modeling

In 3D, a linear elastic solid has at most 21 independent elasticity constants. To reduce this number, the symmetry of the material itself can be exploited.



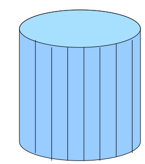
c1	c2	c3	0	0	0
	c4	c5	0	0	0
		c6	0	0	0
			c7	0	0
				c8	0
					c9

orthotropic, 9 coefficients
Symmetry wrt 180°rotations



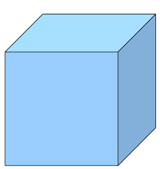
c1	c2	c3	0	0	0
	c1	c3	0	0	0
		c6	0	0	0
			c7	0	0
				c7	0
					c9

orthotropic, horizontally regular, 6 coefficients, Symmetry wrt 180° rotations and 90°rotations about a given axis of symmetry



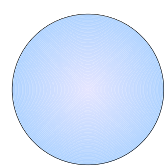
c1	c2	c3	0	0	0
	c1	c3	0	0	0
		c6	0	0	0
			c7	0	0
				c7	0
					(c1−c2)/2

orthotropic, horizontally isotrop ("transverse isotropic"), 5 coefficients
Symmetry wrt 180°rotations and arbitrary rotations about a given axis



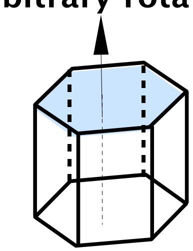
c1	c2	c2	0	0	0
	c1	c2	0	0	0
		c1	0	0	0
			c7	0	0
				c7	0
					c7

regular cubic, 3 coefficients
Symmetry wrt 90°rotations about 3 fixed perpendicular axes



c1	c2	c2	0	0	0
	c1	c2	0	0	0
		c1	0	0	0
			2(c1−c2)	0	0
				2(c1−c2)	0
					2(c1−c2)

isotropic, 2 coefficients
Symmetry wrt arbitrary rotations
$c1 = \lambda + 2\mu$, $c2 = \lambda$



c1	c2	c3	0	0	0
	c1	c3	0	0	0
		c6	0	0	0
			c7	0	0
				c7	0
					2(c1−c2)

hexagonal symmetry, 5 coefficients
Symmetry wrt n x 30°rotations about given axis (c-axis)

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2. A flow law for ice: continuum mechanical modeling

Nye's generalization of Glen's flow law:

Postulate: Cold ice is a density preserving, viscous, heat conducting fluid

Constitutive relation: $\mathbf{T}^E = \check{\mathbf{T}}(\mathbf{D}, T, \text{grad } T) \Longleftrightarrow \mathbf{D} = \check{\mathbf{D}}(\mathbf{T}^E, T, \text{grad } T)$

Assumption 1: The dependence on grad T has never been measured and is hence dropped. Rational Mechanics Modeling gives

$$\mathbf{D} = \beta_1 \mathbf{1} + \beta_2 \mathbf{T}^E + \beta_3 {\mathbf{T}^E}^2 \qquad \beta_1, \beta_2, \beta_3 = \text{fct}(\text{tr } \mathbf{T}^E, \text{tr } {\mathbf{T}^E}^2, \det \mathbf{T}^E, T)$$

Incompressibility: div $\mathbf{v} = 0$ or tr $\mathbf{D} = 0$

$$0 = 3\beta_1 + \beta_3 \text{tr}({\mathbf{T}^E}^2)$$

$$\mathbf{D} = -\beta_3 \text{tr}({\mathbf{T}^E}^2)/3 + \beta_2 \mathbf{T}^E + \beta_3 {\mathbf{T}^E}^2$$

2. A flow law for ice: continuum mechanical modeling

Nye's generalization of Glen's flow law (cntd):

Assumption 2: **D** and $\mathbf{T}^E$ are collinear to each other ($\beta_3 = 0$).

$$\mathbf{D} = \beta_2 \mathbf{T}^E \qquad \beta_2 = \mathrm{fct}(\mathrm{tr}\ \mathbf{T}^E = 0,\ \mathrm{tr}\ {\mathbf{T}^E}^2,\ \det\ \mathbf{T}^E,\ T)$$

Assumption 3: **D** does not depend on det $\mathbf{T}^E$

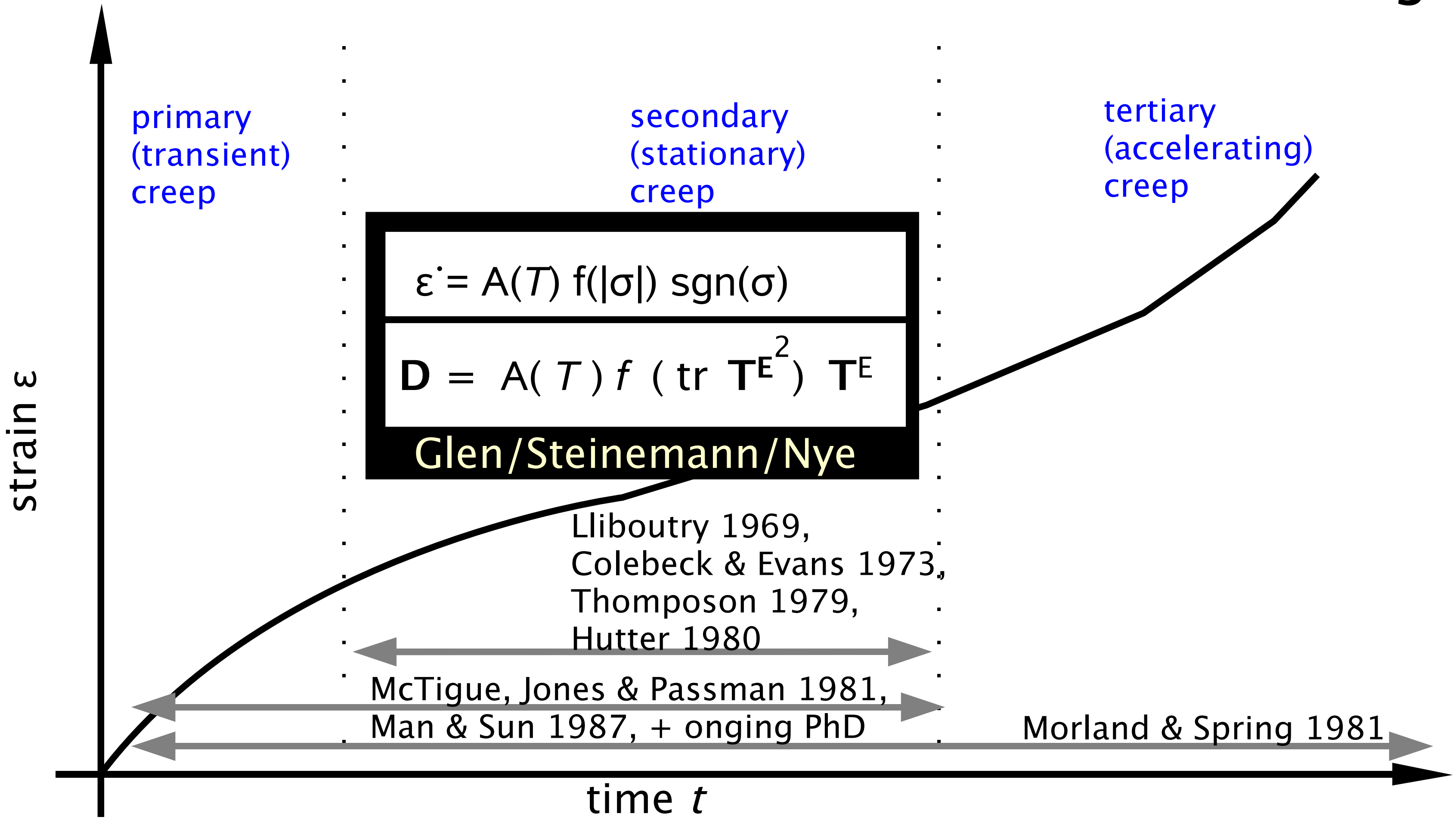
$$\mathbf{D} = \beta_2 \mathbf{T}^E = \beta_2(\mathrm{tr}\ {\mathbf{T}^E}^2,\ T)\ \mathbf{T}^E$$

Assumption 4: β_2 can be factorized as $\beta_2(\mathrm{tr}\ {\mathbf{T}^E}^2,\ T) = A(T)\, f\,(\mathrm{tr}\ {\mathbf{T}^E}^2)$

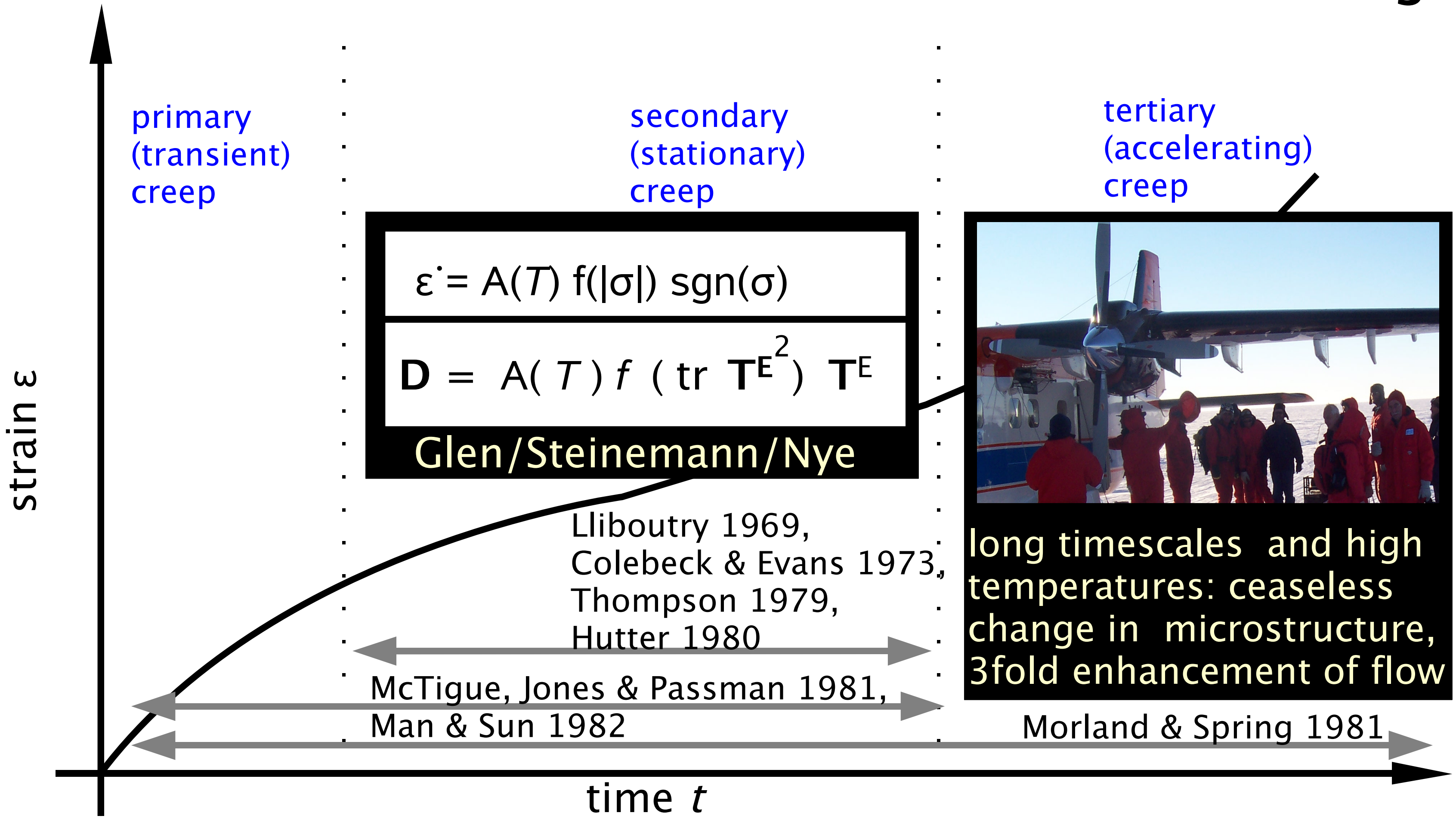
$$\mathbf{D} = A(T)\, f\,(\mathrm{tr}\ {\mathbf{T}^E}^2)\ \mathbf{T}^E$$

3D generalization of the flow law of Glen & Steinemann (Nye 1952)

2. A flow law for ice: continuum mechanical modeling



2. A flow law for ice: continuum mechanical modeling

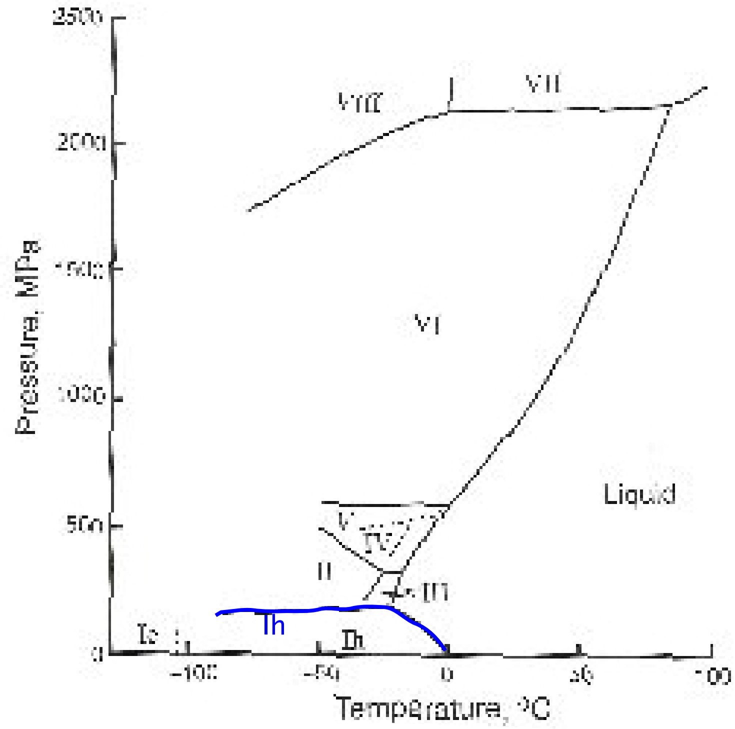


3. Microscale processes beyond secondary creep

Properties of H_20

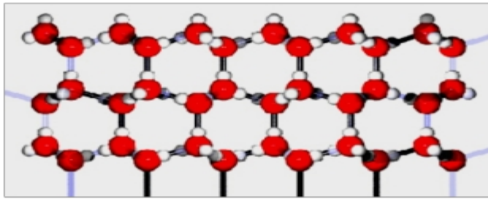
Water has the greatest diversity (polymorphism) of solid phases over all known substances:

- 2 amorphous phases (lacking crystalline structure)
- 16 crystalline phases (ice Ih, Ic, II – XV)



Ice Ih possesses hexagonal symmetry

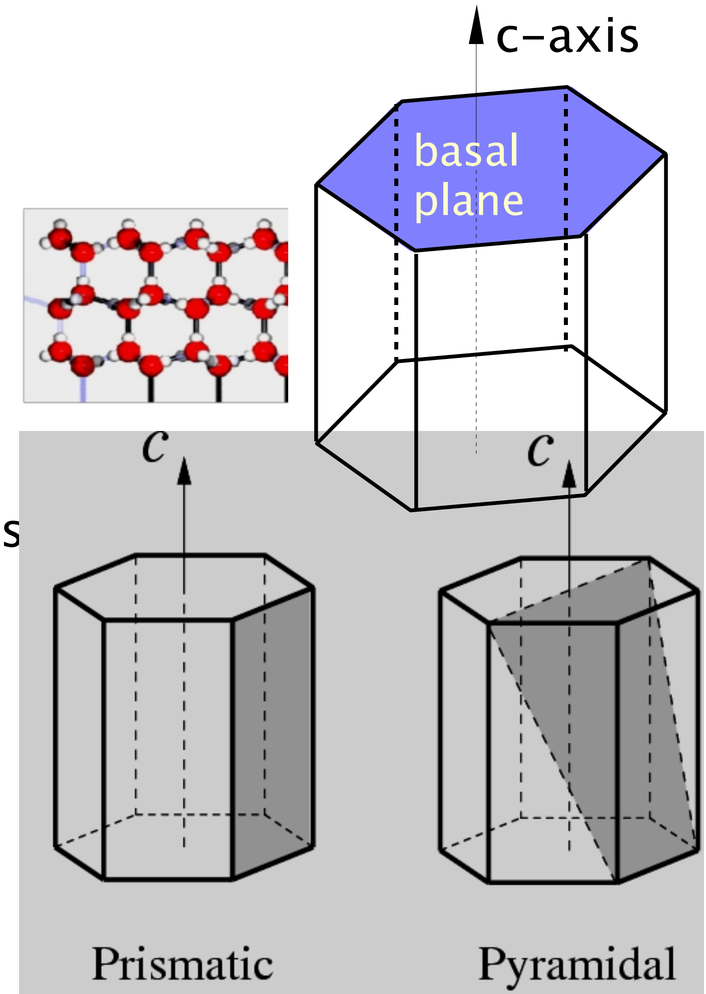
- atomic packing factor: < 34%



3. Microscale processes beyond secondary creep

Microstructure of ice Ih

- hexagonal symmetry
- concentration of molecules in *basal planes*
- weak O=O bonding in between basal planes ("hard glide" along pyramidal/prismatic planes
- strong O=O bonding within the basal planes ("easy glide" along basal planes)
- c–axis: perpendicular to basal planes



3. Microscale processes beyond secondary creep

Microstructure of ice Ih

strong O=O bonding within the basal planes (”easy glide” along basal planes)

- slip resistance along basal planes is up to 60 times smaller than in other slip systems (210 K < T < 273.15 K)

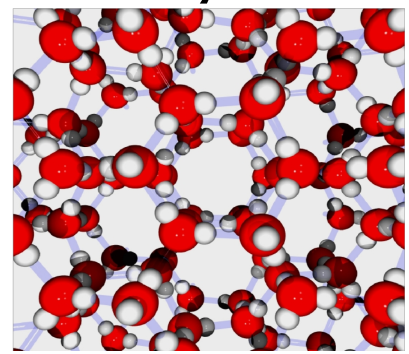
- the ”deck of cards” analogy dates back to McConell (1891)

[redacted] the crystal behaved as if it consisted of an infinite number of indefinitely thin sheets of paper, normal to the optic axis, attached to each other by some viscous substance which allowed one to slide over the next with great difficulty. This comparison proved to be the key to the whole question of the plasticity of a crystal of ice.

- slip along basal planes takes place via dislocation glide and is regarded as the dominant deformation mechanism

3. Microscale processes beyond secondary creep

Dislocations and other imperfections: Hypothetical vs. real crystals

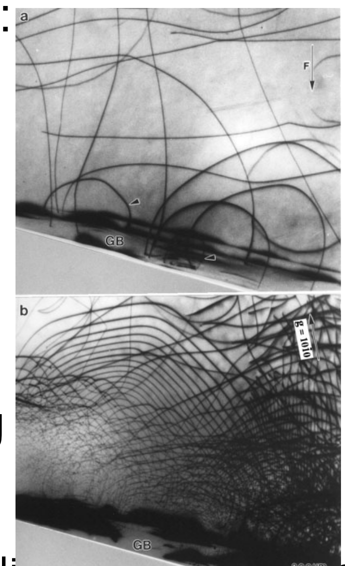


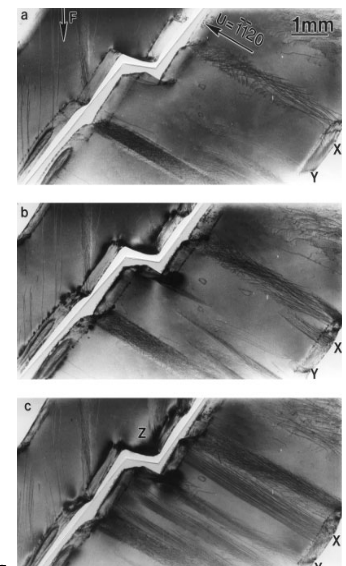
- Distribution of hydrogens in the oxygen lattice: 2 hydrogen nuclei close to any oxygen but only one per joining line (Bernal-Fowler rule)
  Violation of these rules: point defects (Bjerrum)

- Discontinuity/offset in the crystal structure: line (1d) / plane (2d) /gross (3d) defects

  line defects (1d): dislocations

  dislocation density ρ_d (total length of line defect per unit volume [l^{-2}]) evolves in time and can lead to strain softening/hardening behavior of ice

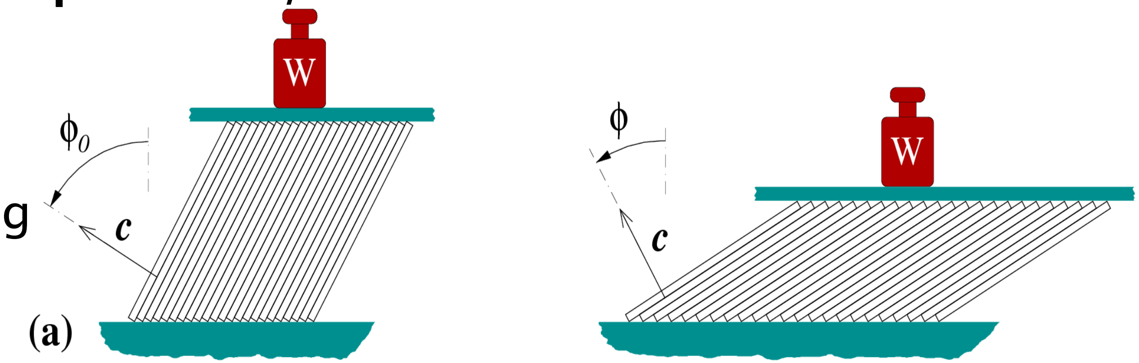




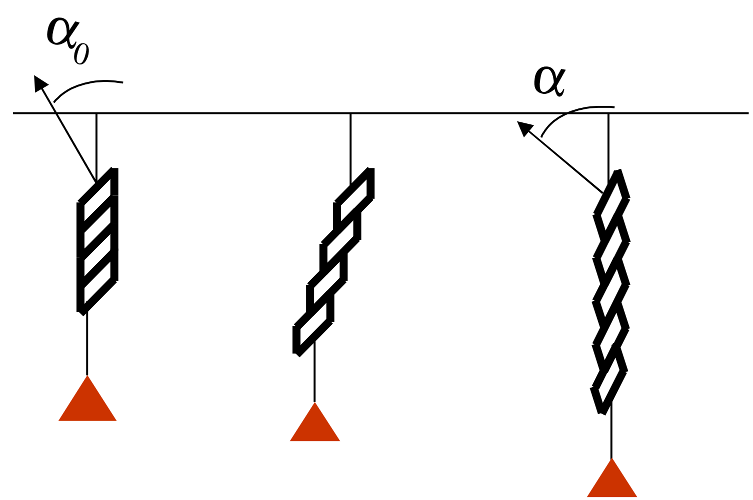
3. Microscale processes beyond secondary creep

c-axis rotation under compression / tension

towards the axis of loading



away from the axis of loading



3. Microscale processes beyond secondary creep

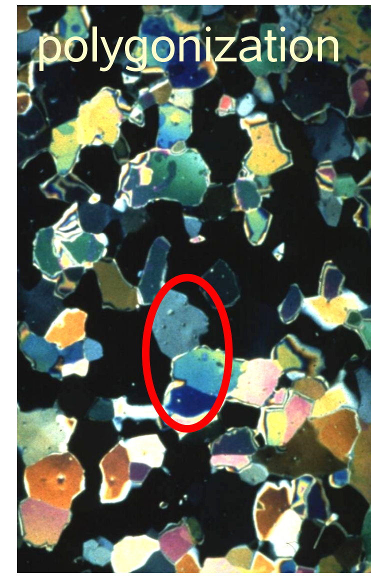
measuring c-axis rotation

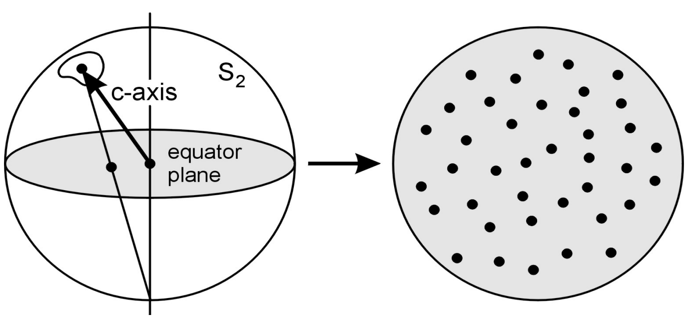
thin sections under crossed polarizers

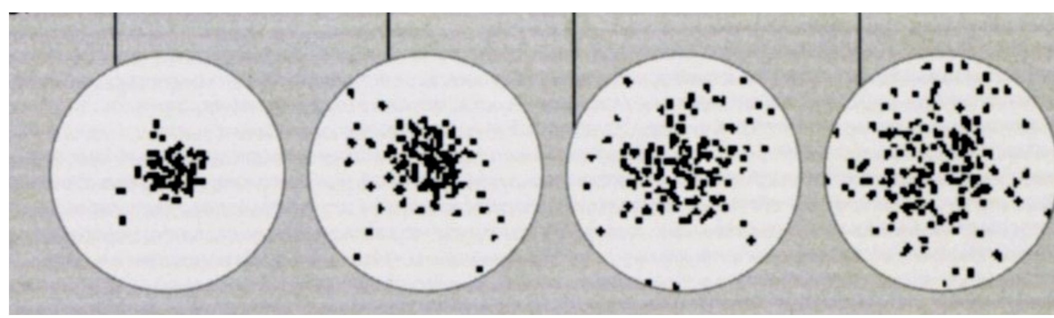
- crystals rotate incoming polarized light depending on c-axis orientation

- differently oriented crystals appear with different colors

- orientations are plotted in Schmidt diagrams







3. Microscale processes beyond secondary creep

Classification of microscale deformation mechanisms

lattice mechanisms: relate to the behavior of the crystalline structure (c-axis evolution)

”fabric”

boundary mechanisms: act at the grain boundaries and relate to grain size (Grain boundary migration, nucleation, recovery, polygonization, ...)

”texture”

crystal-size dependent isotropic rheology:
Barnes (1972), Goldsby & Kohlstedt (1997)

3. Microscale processes beyond secondary creep

Homogenization of microscopic deformation within a RVE

Consideration of basal glide alone during deformation:

How to deal with geometric misfits occurring between neighboring crystals?

- Taylor's hypothesis (1938, "Plastic strain in metals"):
  all crystals in an RVE suffer the same strain now discarded for polycrystalline ice

- Sachs' hypothesis (1928, "Zur Ableitung einer Fliessbedingung" *[On the derivation of a yield criterion]*):
  all crystals in the RVE suffer the same stress

- VPSC (ViscoPlastic Self Contained; Castelnau, Duval, Lipenkov,... ~1996):
  combining Taylor and Sachs: stress equilibrium and strain compatibility are recursively satisfied
  difficulties when formulating a macroscopic flow law
  not extendable to non-liner stress-deformation relations