

Micromechanical modeling of near β -Ti alloys:

Effect of elastic anisotropy on the elastic-viscoplastic transition, incompatibility stresses and slip activity

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Near β -Ti alloys...

Ti-5553

Ti-17

Ti-10-2-3

Chemical composition (w%)

	Al	Mo	V	Fe	Sn	Zr	Cr
Ti-5553	5	5	5	0.5	0	0	3
Ti-17	5	4	0	0	2	2	4
Ti-10-2-3	3	0	10	2	0	0	0

α -elements

β -elements

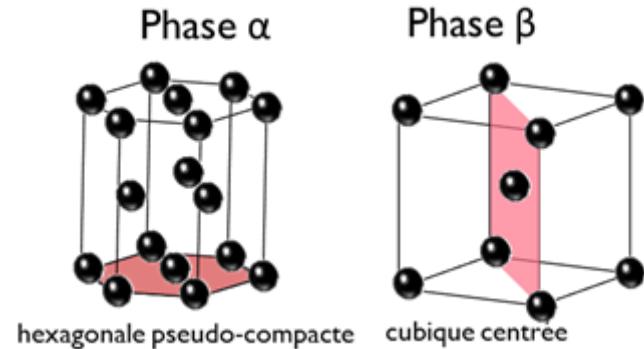
... for Airframe Applications



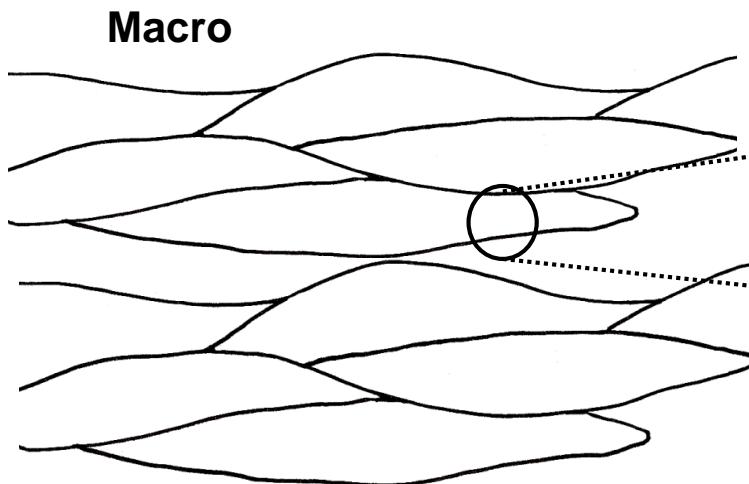
Landing
gears



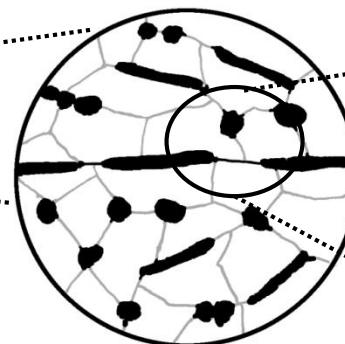
Rotor
Systems



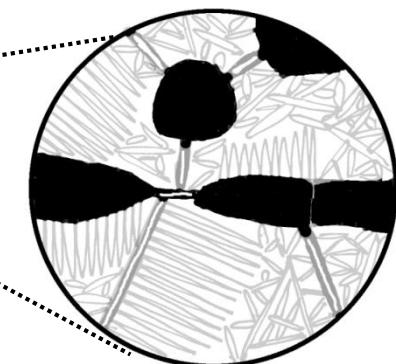
In-service microstructure : complex and multi-scale*



Meso



Micro



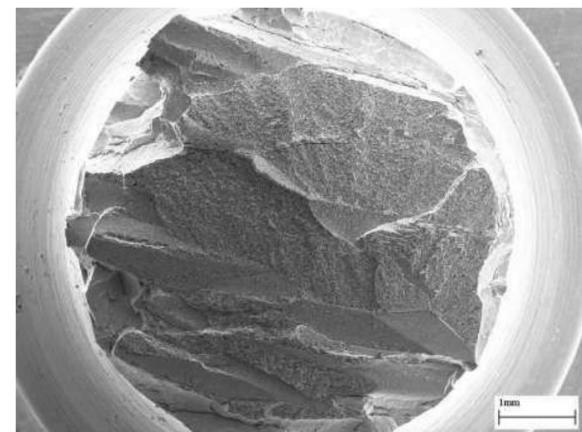
40% of β res phase revealing
Millimeter large prior β grains

Primary α_p
nodules

Secondary α_s
Precipitation

Strong elastic
anisotropy of
both β and α
phases

Influence the
Stress distribution
under fatigue loading



Fracture surface in Ti-5553
[N. Clément, 2010]

*M.R. Chini et al. (2016) in Proceedings of the 13th World Conference on Titanium

Our purpose

→ To evaluate the role of the elastic anisotropy on both the overall mechanical behavior and the local behavior

1. First, considering a 100% equiaxed β microstructure

β elastic anisotropy

crystallographic β texture

- 1) Uniaxial, multiaxial and reversible loading, Bauschinger stress
- 2) Incompatibility stresses and slip activity

2. Then, considering an equiaxed nodular microstructure α - β

Based on:

An affine Elasto-Viscoplastic Self-Consistent model (EVPSC)

- Elasto-viscoplastic coupling (Translated fields)
- Non linear viscoplastic flow rule (affine approximation)

Outline

- 1) Which Elastic Constants describe at best
the β -phase elastic behavior ?
- 2) Our affine EVPSC model
to capture the elasto-viscoplastic transition
- 3) The macroscopic elasto-viscoplastic and the local
behaviors in a 100% β -Ti alloy:
 - β elastic anisotropy
 - crystallographic β texture
- 4) The tensile elasto-viscoplastic behavior, slip activities and
local plastic strain in nodular microstructure α - β

Literature reports A coeff. ranging from 1.4 to 8.3 for the β phase

References	C (GPa)			A*	Ti alloy	Method
	C11	C12	C44			
Fréour et al. (2005)	174	116	41	1.4	Ti17	Xray diffraction + inverse SC
Fréour et al. (2011)	167	115	44	1.7	Ti17	Xray diffraction +inverse SC
Nejezchlebova et al. (2016)	138	102.2	42.5	2.37	Single crystal LCB	Ultrasound+Hill model
Martin et al. (2012)	100	70	36	2.4	Ti17-Ti5553	Fitted from experiments
Petry et al. (1991)	134	110	36	3	Pure	Phonon dispersion
Brandes et al. (1992)	134	110	55	4.6	Pure	?
Fisher & Dever (1970)	99	85	33.6	4.8	Pure	?
Kim et al. (2009)	135	113	54.9	5	Ti6-2-4-2	Line focus acoustic microscopy
Ledbetter et al. (2004)	97.7	82.7	37.5	5	Pure	Resonant ultrasound spectroscopy
Raghunathan et al. (2007)	140	128	50	8.3	Ti10-2-3	Xray diffraction +inverse SC

$$* A = \frac{2C_{44}}{C_{11} - C_{12}}$$

Only 3 sets of elastic constants give the β -Ti Young Modulus

(Lhadi et al, 2018 Int. J. Plast.)

References	C (GPa)			A*	Ti alloy	Method	Effective Young's modulus (GPa)**
	C11	C12	C44				
Fréour et al. (2005)	174	116	41	1.4	Ti17	Xray diffraction + inverse SC	98.6
Fréour et al. (2011)	167	115	44	1.7	Ti17	Xray diffraction + inverse SC	98.4
Nejezchlebova et al. (2016)	138	102.2	42.5	2.37	Single crystal LCB	Ultrasound+Hill model	83.8
Martin et al. (2012)	100	70	36	2.4	Ti17-Ti5553	Fitted from experiments	69.4
Petry et al. (1991)	134	110	36	3	Pure	Phonon dispersion	66.6
Brandes et al. (1992)	134	110	55	4.6	Pure		85.8
Fisher & Dever (1970)	99	85	33.6	4.8	Pure		52.8
Kim et al. (2009)	135	113	54.9	5	Ti6-2-4-2	Line focus acoustic microscopy	83.7
Ledbetter et al. (2004)	97.7	82.7	37.5	5	Pure	Resonant ultrasound spectroscopy	57.5
Raghunathan et al. (2007)	140	128	50	8.3	Ti10-2-3	Xray diffraction + inverse SC	67.2

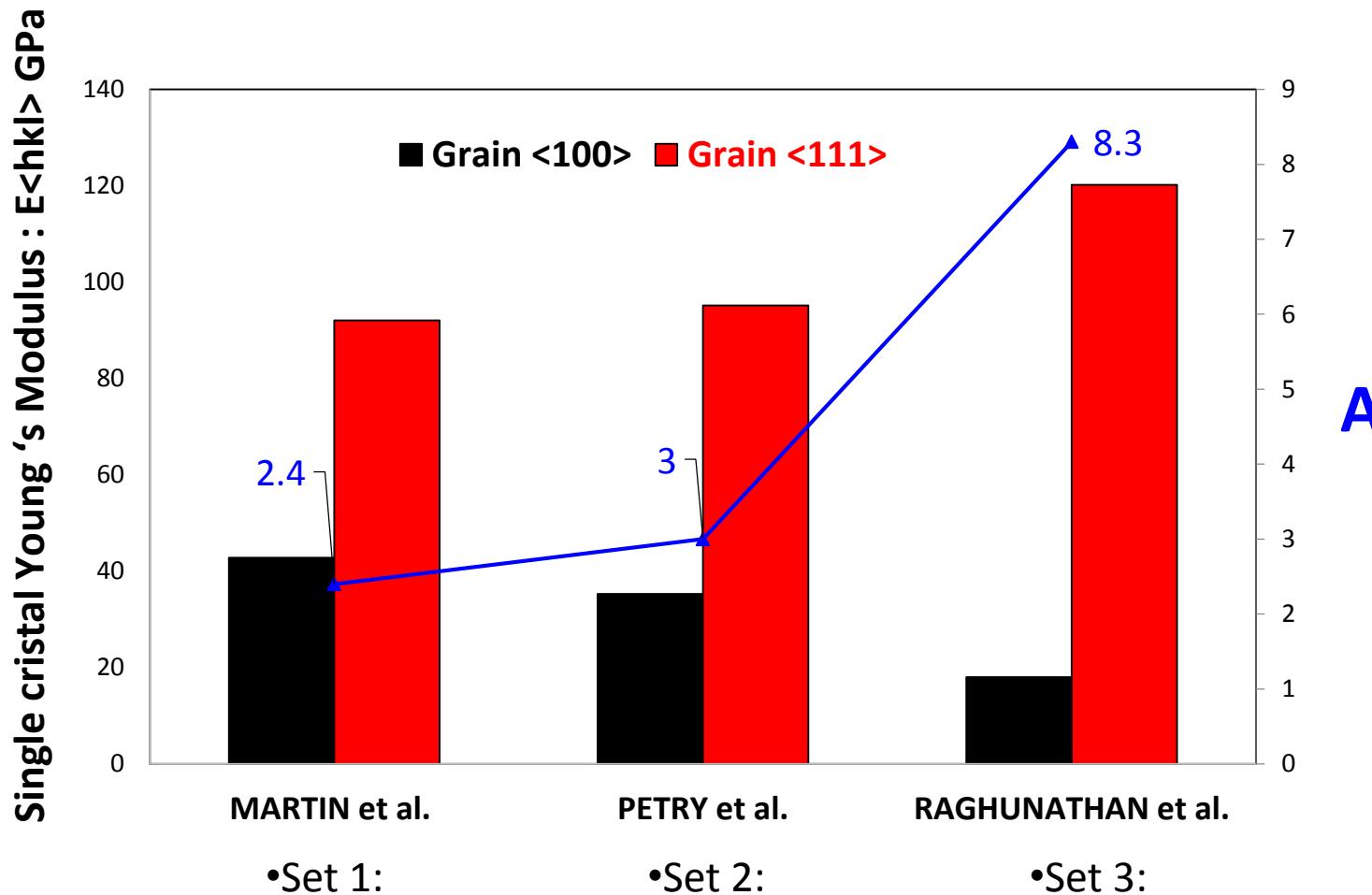
**Polycrystal: spherical grains and random texture

Effective Young's modulus of Ti-17 : 68 GPa
(A. Settefrati, 2012)

These 3 sets of elastic constants give large differences in :

-Extreme $E_{\langle hkl \rangle}$ variations : $E_{\langle 100 \rangle}$ vs $E_{\langle 111 \rangle}$

- Anisotropy coefficients : A

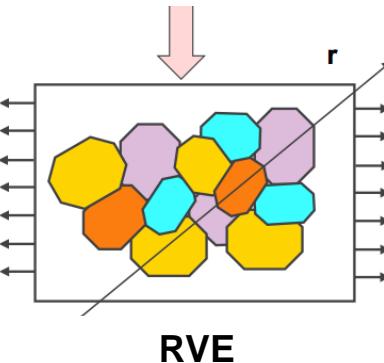


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- 2) Our affine EVPSC model to capture the elasto-viscoplastic transition
 - Mareau and Berbenni (2015) *Int. J. Plast.*
 - Lhadi et al. (2018) *Int. J. Plast.*
- 3) The macroscopic elasto-viscoplastic and the local behaviors in a 100% β -Ti alloy:
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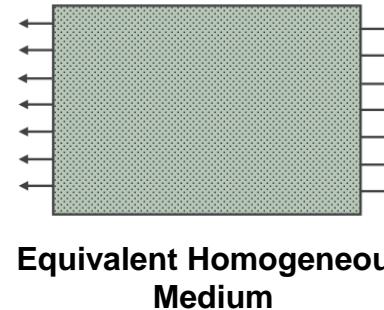
Motivation: Micro-Macro homogenization scale transitions for elasto-viscoplasticity

Real material



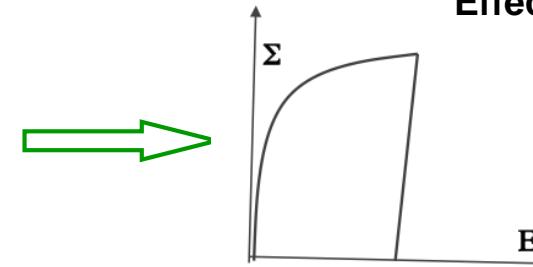
RVE

Scale transition



Equivalent Homogeneous Medium

Effective behavior



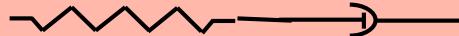
$$\text{Elasticity} \quad \boldsymbol{\sigma} = \mathbf{C} : \boldsymbol{\varepsilon}$$



$$\boldsymbol{\Sigma} = \mathbf{C}^{\text{eff}} : \mathbf{E} \quad \text{quite easy}$$

Elasto-viscoplasticity

$$\dot{\boldsymbol{\varepsilon}} = \mathbf{S} : \dot{\boldsymbol{\sigma}} + \mathbf{m} : \boldsymbol{\sigma}$$



difficult

- Inhomogeneous material and linear (or linearized) behavior
- Space-Time coupling due to different time derivation orders



Non conventional solution: Translated fields

Field equations for elasto-viscoplastic behavior

$$\dot{\underline{\varepsilon}} = \dot{\underline{\varepsilon}}^e + \dot{g}(\underline{\sigma})$$

$$\underline{\operatorname{div}} \dot{\underline{\sigma}} = 0$$

$$\underline{\operatorname{div}} \underline{\sigma} = 0$$

$$\dot{\underline{\varepsilon}} = \nabla^s \dot{\underline{u}}$$

$$\dot{\underline{u}}^d = \dot{\underline{E}} \cdot \underline{x}$$

with:

$$\begin{cases} \dot{\underline{\varepsilon}}^e = \underline{s} : \dot{\underline{\sigma}} \\ \dot{\underline{\varepsilon}}^{vp} = g(\underline{\sigma}) \end{cases}$$

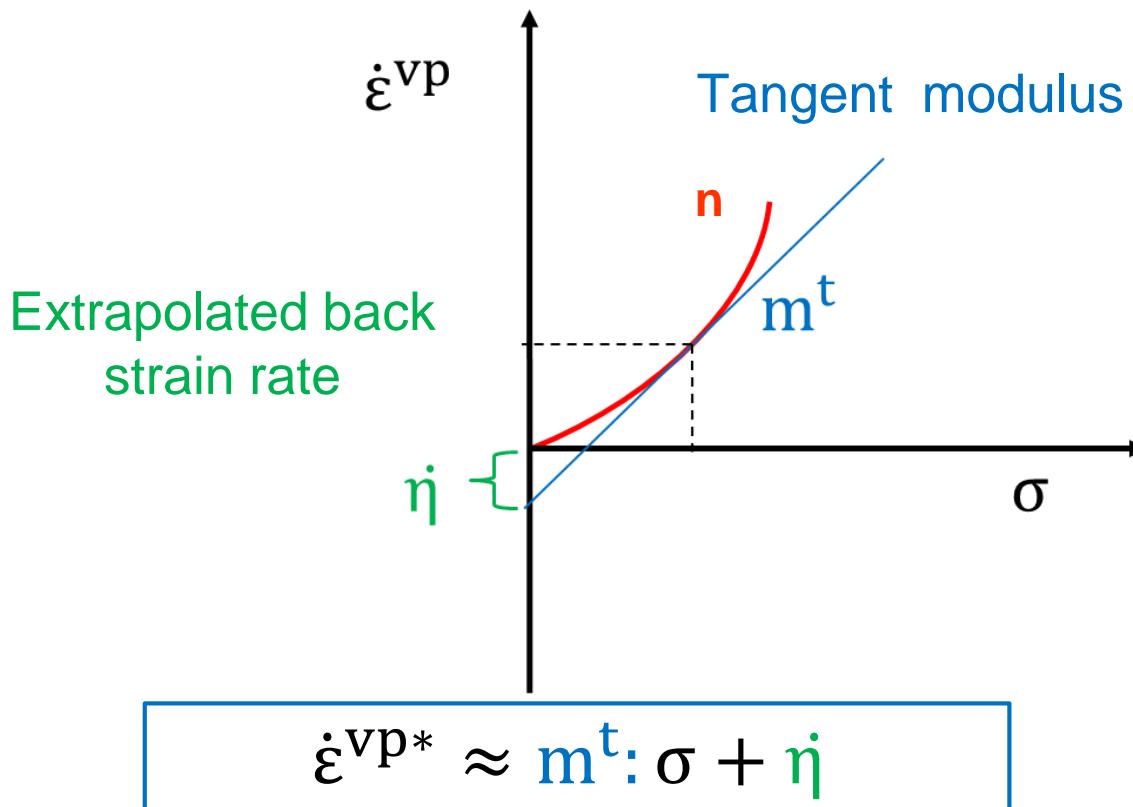


Viscoplasticity:
non linear function of stress

Need to be approximated

Viscoplastic flow rule - affine linearization

(Masson et al. 2000)

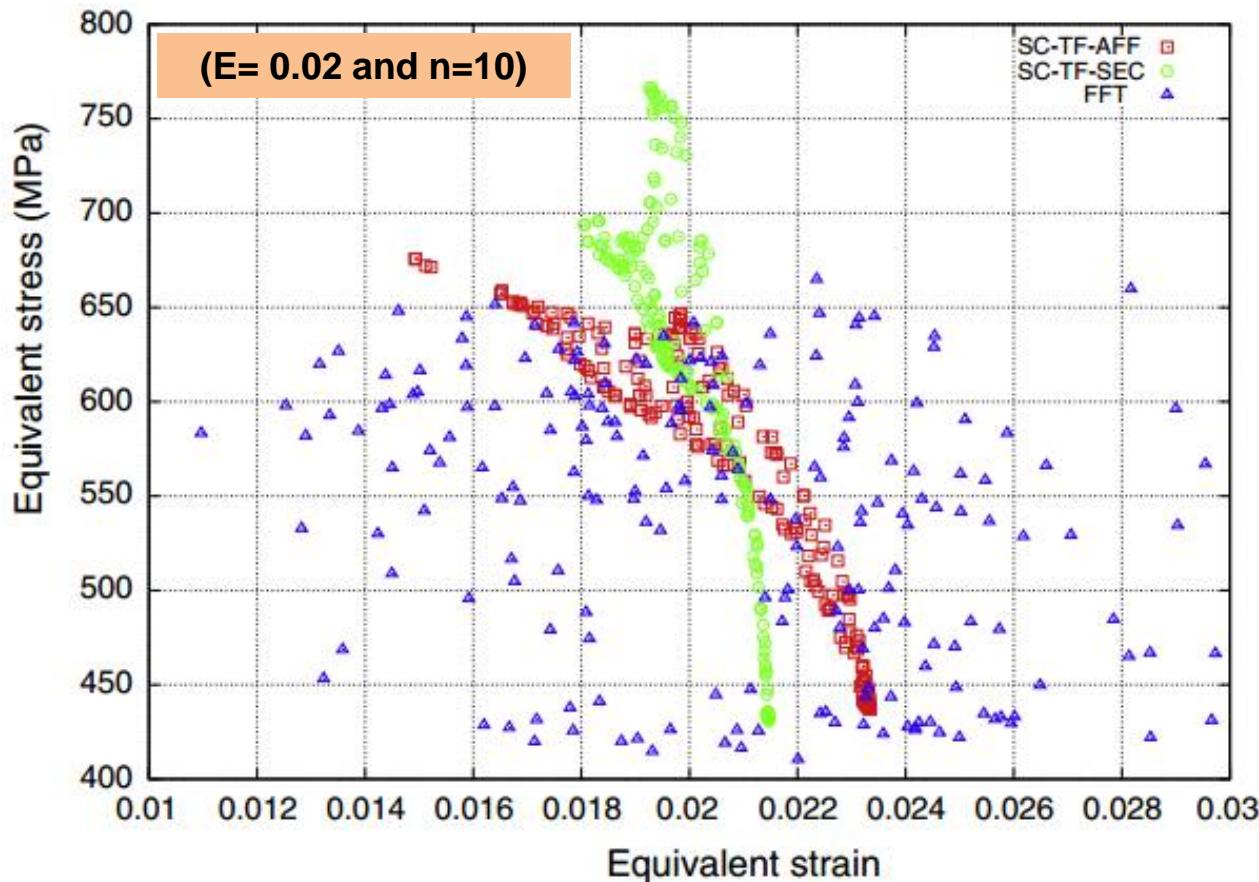


Good description of the overall response of heterogeneous materials : close to FFT calculations

*-Mareau and Berbenni (2015) Int. J. Plast.

-Berbenni et al. (2015) Comptes Ren. Méca.

Viscoplastic flow rule - affine linearization



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Integral equation for elasto-viscoplastic behavior

$$\dot{\boldsymbol{\varepsilon}} = \dot{\boldsymbol{E}} - \boldsymbol{\Gamma}^C * (\delta \boldsymbol{c} : \dot{\boldsymbol{\varepsilon}}^e) - \boldsymbol{\Gamma}^{B_t} * (\delta \boldsymbol{b}_t : \dot{\boldsymbol{\varepsilon}}^{vp} - \boldsymbol{b}_t : \dot{\boldsymbol{\eta}}) + (\boldsymbol{\Gamma}^C : \boldsymbol{C} - \boldsymbol{\Gamma}^{B_t} : \boldsymbol{B}_t) * \dot{\boldsymbol{\varepsilon}}^{vp}$$

Using the translated field method, **the interaction law for 1-site self-consistent model** writes:

$$\begin{aligned}\dot{\boldsymbol{\sigma}} = & \boldsymbol{c} : \boldsymbol{A}^C : (\boldsymbol{S}^e : \dot{\boldsymbol{\Sigma}} + \dot{\boldsymbol{E}}^{vp,e}) - \boldsymbol{c} : \dot{\boldsymbol{\varepsilon}}^{vp} + \boldsymbol{c} : \boldsymbol{A}^C : \boldsymbol{\Gamma}_l^{B_t} : (\boldsymbol{b}_t : \dot{\boldsymbol{\eta}} + \boldsymbol{B}_t^e : \dot{\boldsymbol{N}}^e) \\ & + \boldsymbol{c} : \boldsymbol{A}^C : \boldsymbol{\Gamma}_l^C : (\delta \boldsymbol{c} : \dot{\boldsymbol{\varepsilon}}^{vp} + \boldsymbol{c} : \boldsymbol{A}^C : (\langle \dot{\boldsymbol{\varepsilon}}^{vp} \rangle - \dot{\boldsymbol{E}}^{vp,e})) \\ & - \boldsymbol{c} : \boldsymbol{A}^C : \boldsymbol{\Gamma}_l^{B_t} : (\delta \boldsymbol{b}_t : \dot{\boldsymbol{\varepsilon}}^{vp} - \boldsymbol{b}_t : \boldsymbol{A}^{B_t} : (\boldsymbol{M}_t^e : \boldsymbol{\Sigma} + \dot{\boldsymbol{N}}^e - \langle \dot{\boldsymbol{\varepsilon}}^{vp} \rangle)) \\ & + \boldsymbol{c} : \boldsymbol{A}^C : (\boldsymbol{\Gamma}_l^C : \boldsymbol{C}^e - \boldsymbol{\Gamma}_l^{B_t} : \boldsymbol{B}_t^e) : (\dot{\boldsymbol{\varepsilon}}^{vp} - \boldsymbol{A}^{B_t} : \langle \dot{\boldsymbol{\varepsilon}}^{vp} \rangle) \\ & - \boldsymbol{c} : \boldsymbol{A}^C : (\boldsymbol{\Gamma}_l^C : \boldsymbol{C}^e - \boldsymbol{\Gamma}_l^{B_t} : \boldsymbol{B}_t^e) : (\boldsymbol{A}^{B_t} : \boldsymbol{\Gamma}_l^{B_t} : (\boldsymbol{b}_t : \dot{\boldsymbol{\eta}} - \boldsymbol{B}_t^e : \dot{\boldsymbol{N}}^e))\end{aligned}$$

Application for :

- FCC crystalline material (Mareau and Berbenni, 2015 Int. J. Plast.)
- Near β -Ti alloys (Lhadi et al, 2018 Int. J. Plast.)
- Pure α -Ti (Amouzou et al, 2016 Int. J. Plast.)

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- 2) Our affine EVPSC model
to capture the elastic-viscoplastic transition
- 3) **The macroscopic elasto-viscoplastic and the local behaviors in a 100% equiaxed β -Ti:**
 - β elastic anisotropy : A = 2.4, 3 and 8.3
 - crystallographic β texture :
Random or (60% <111> and 40% <100>)
close to as observed for forged β -Ti phase
- 4) The tensile elasto-viscoplastic behavior, slip activities and
local plastic strain in nodular microstructure α - β

Single-crystal viscoplastic law of β -phase

- Slip rate*

$$\dot{\gamma}^s = \eta^s \frac{\langle |\tau^s - x^s| - r^s \rangle^n}{K}$$

$$\eta^s = \text{sign}(\tau^s - x^s)$$

- Kinematic hardening

$$x^s = c^s \alpha^s$$

$$\dot{\alpha}^s = (\eta^s - d\alpha^s) |\dot{\gamma}^s|$$

- Isotropic hardening

$$r^s = \tau_c^s + bQ \sum_r h_{sr} \rho^r$$

$$\dot{\rho}^r = (1 - b\rho^r) |\dot{\gamma}^r|$$

* Méric et al. (1991), Méric & Cailletaud (1991)

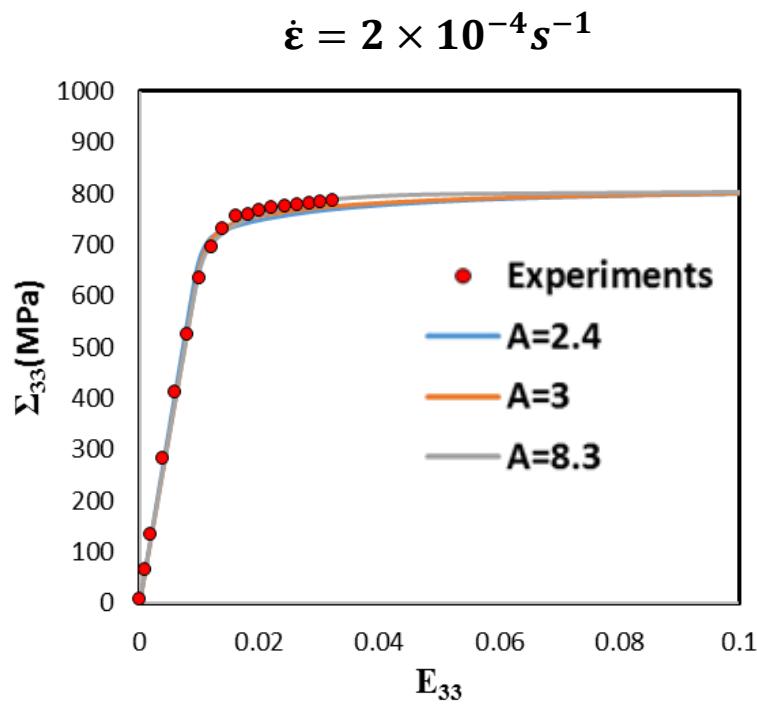
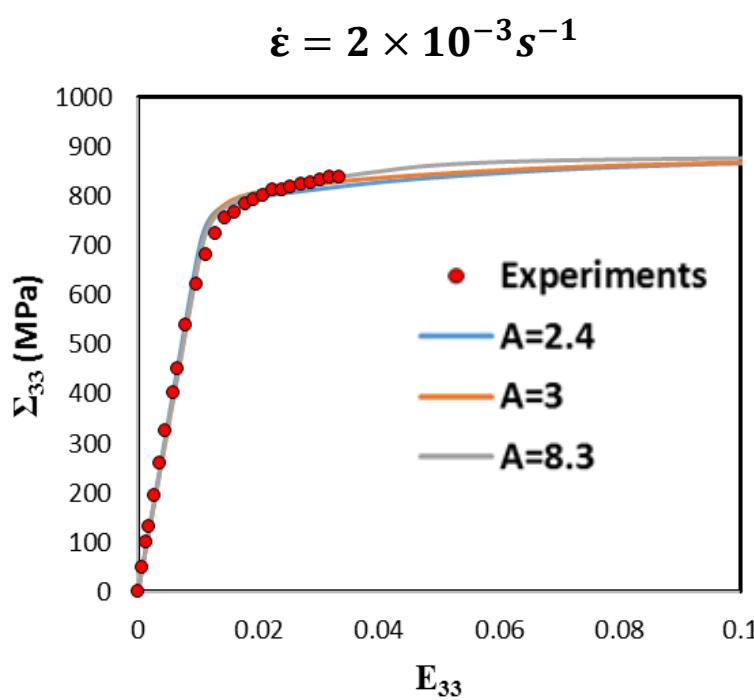
Fitted parameters from experiments a 100% β Ti-17 (from literature**)

Neglected in tensile test simulations

	n	$K(\text{MPa} \cdot \text{s}^{1/n})$	$\tau_c(\text{MPa})$	$c(\text{MPa})$	d	Q
{110} <111>	20	300	113	200	0	0
{112} <111>	20	300	113	200	0	0
{123} <111>	20	300	123	400	0	0

** PhD Thesis of Martin G. (2012) Ecole Nationale Supérieure des Mines de Paris

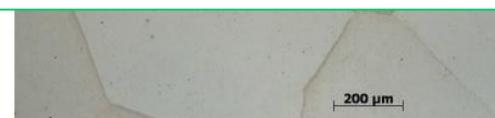
Effect of elastic anisotropy on the macroscopic elastic-viscoplastic behavior



- Experimental data: Ti-17 100% beta- isotropic texture and spherical grains [A. Settefrati, 2012, T. Duval, 2013, G. Martin, 2012]

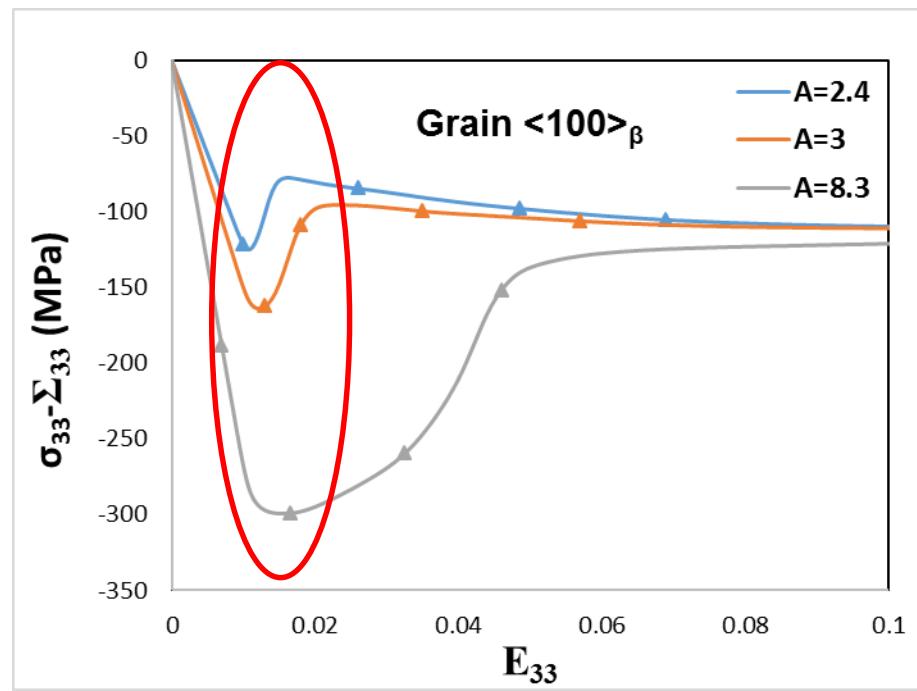
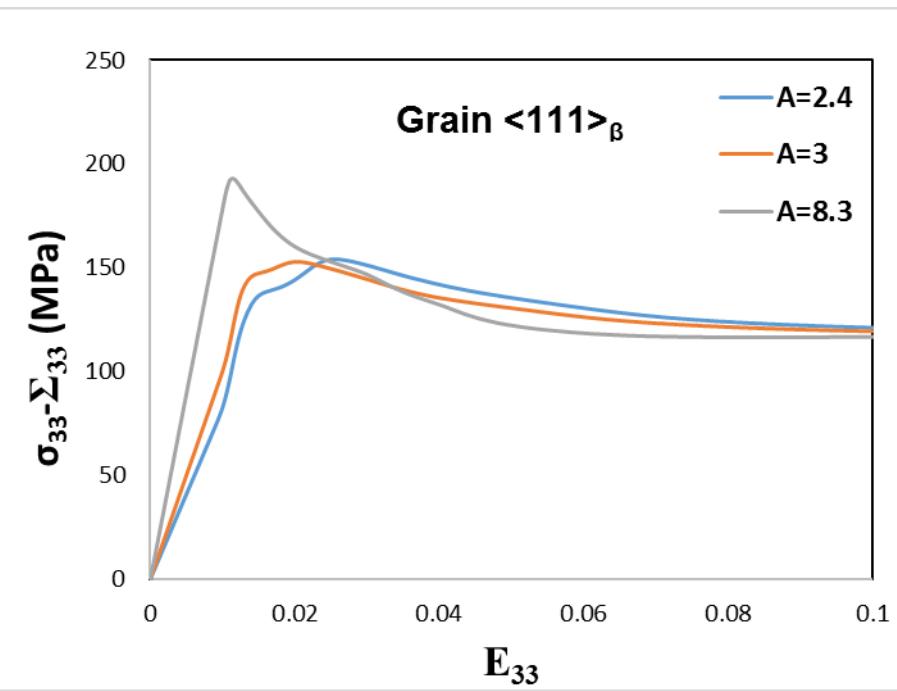


Heat treatment at 920°C-15 min + Quenching



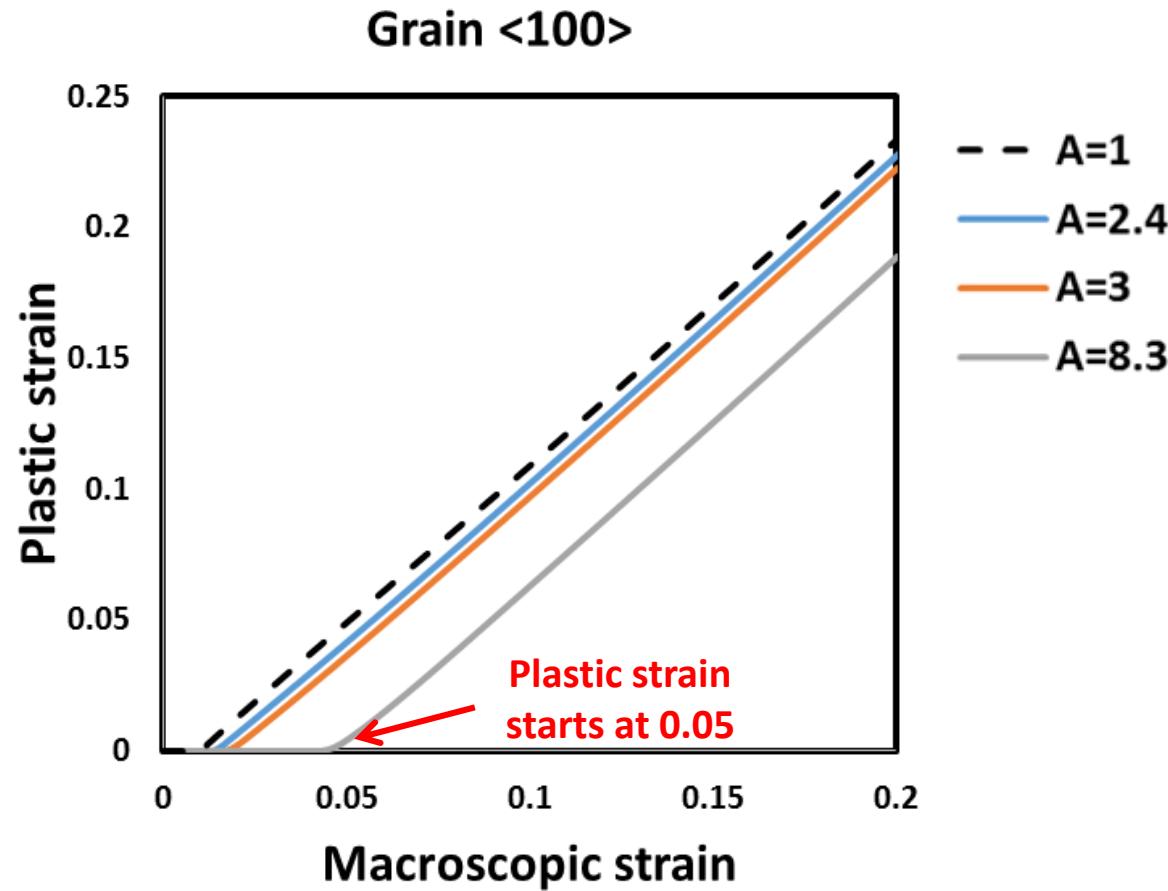
Effect of elastic anisotropy on Incompatibility Stresses: grains $<111>_{\beta}$ and $<100>_{\beta}/\text{TD}$

$$\dot{\varepsilon} = 2 \times 10^{-3} \text{s}^{-1}$$

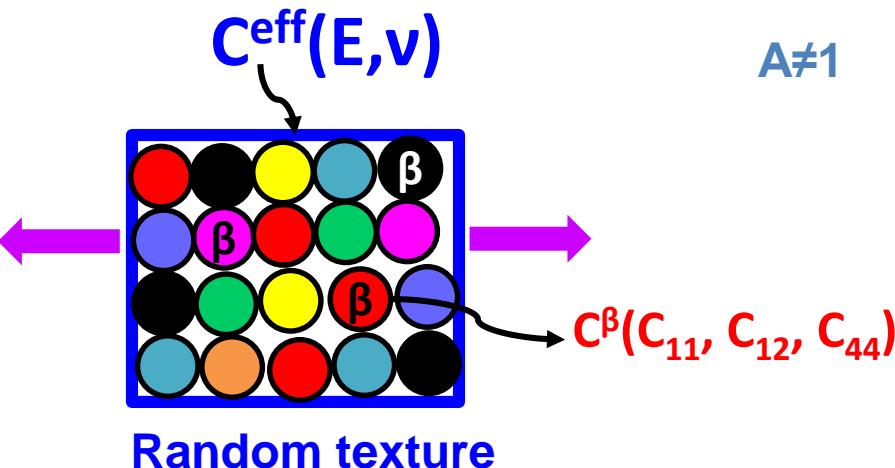


Lhadi S., Berbenni S., Gey N., Richeton T., Germain L., 2018. Micromechanical modeling of the effect of elastic and plastic anisotropies on the mechanical behavior of β -Ti alloys. International Journal of Plasticity. 109 (2018) 88-107.

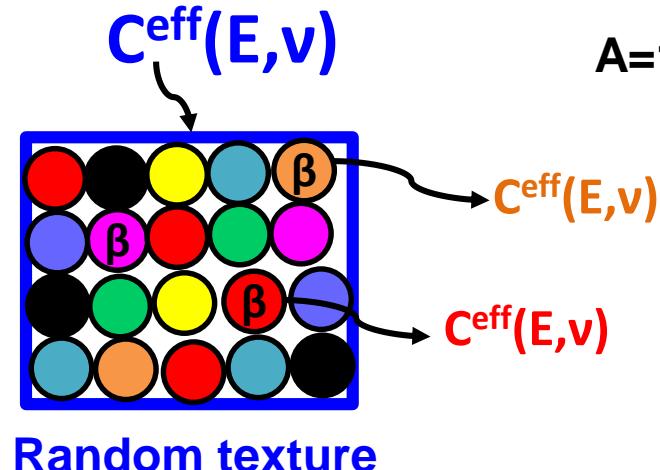
Incompatibility stresses affect plastic strain of grain $<100>$ for $A=8.3$



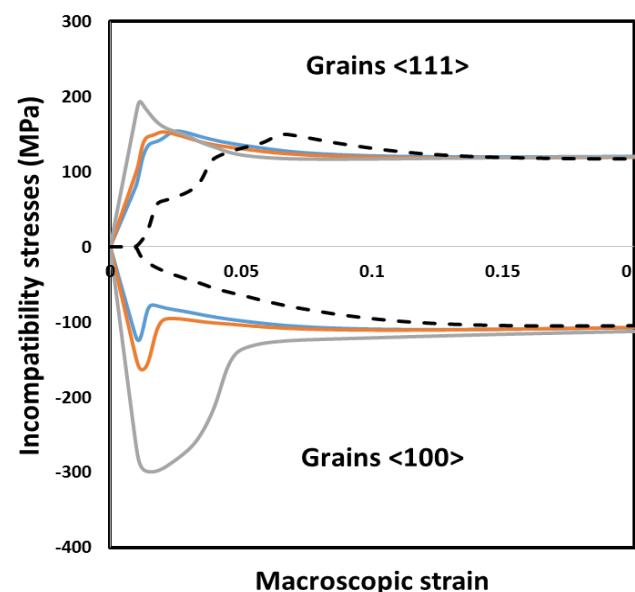
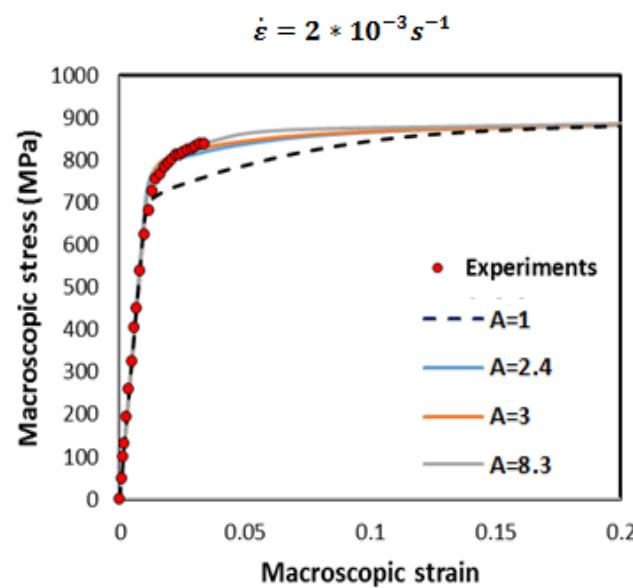
Anisotropic elasticity VS isotropic elasticity ($A=1$)



$A \neq 1$



$A = 1$



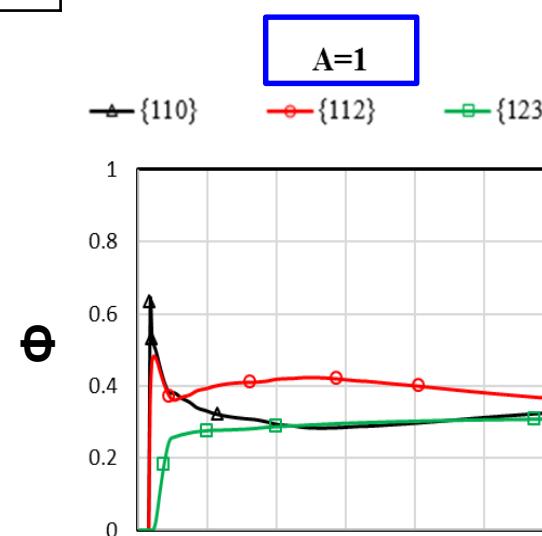
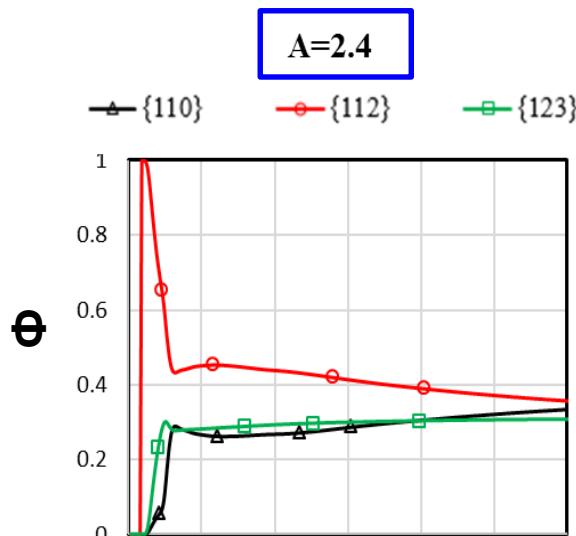
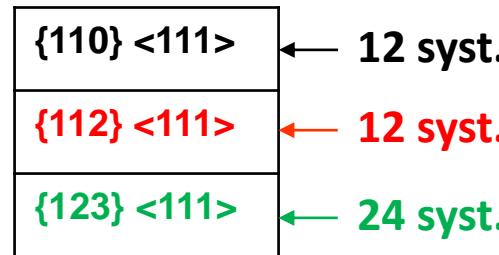
Anisotropic elasticity VS isotropic elasticity (A=1) (2)

Relative activity of a β -phase slip family:

$$\Phi = \frac{\sum_{g=1}^{ng} \sum_{s=p}^q f_g |\dot{\gamma}_g^s|}{\sum_{g=1}^{ng} \sum_{s=1}^{ns} f_g |\dot{\gamma}_g^s|}$$

Slip rate

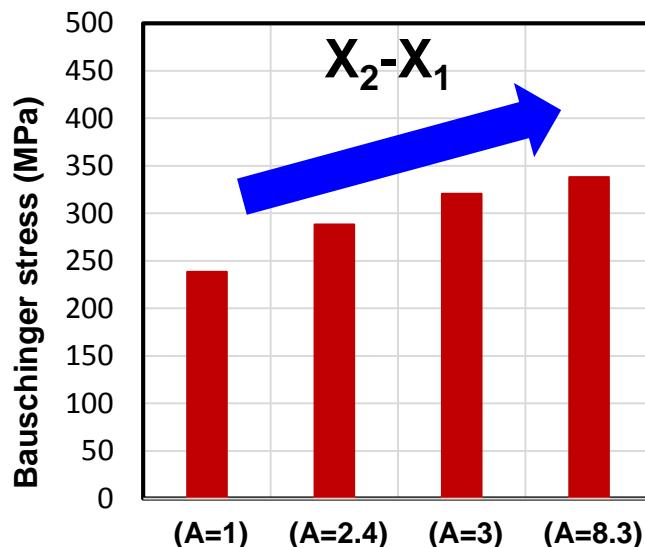
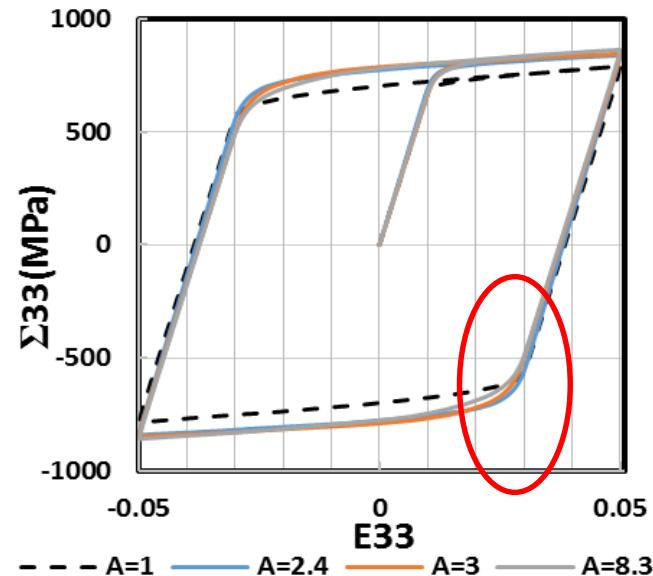
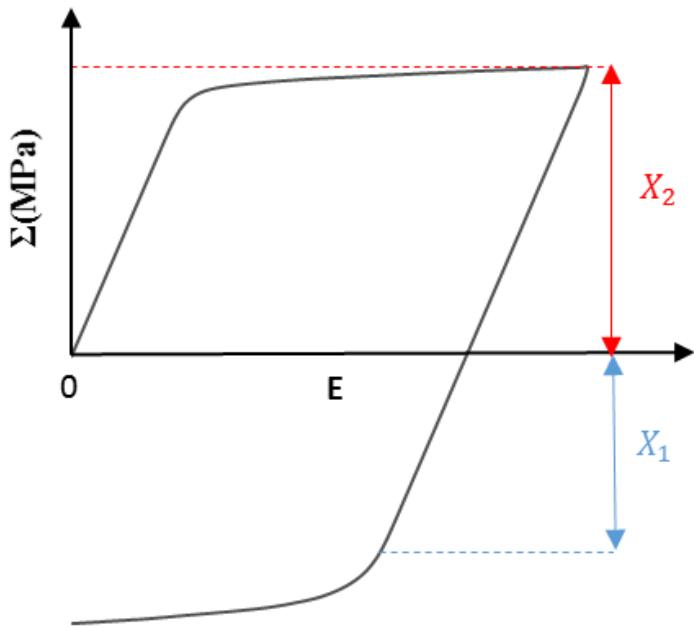
$$\dot{\gamma}^s = \eta^s \frac{(|\tau^s - x^s| - r^s)^n}{K}$$



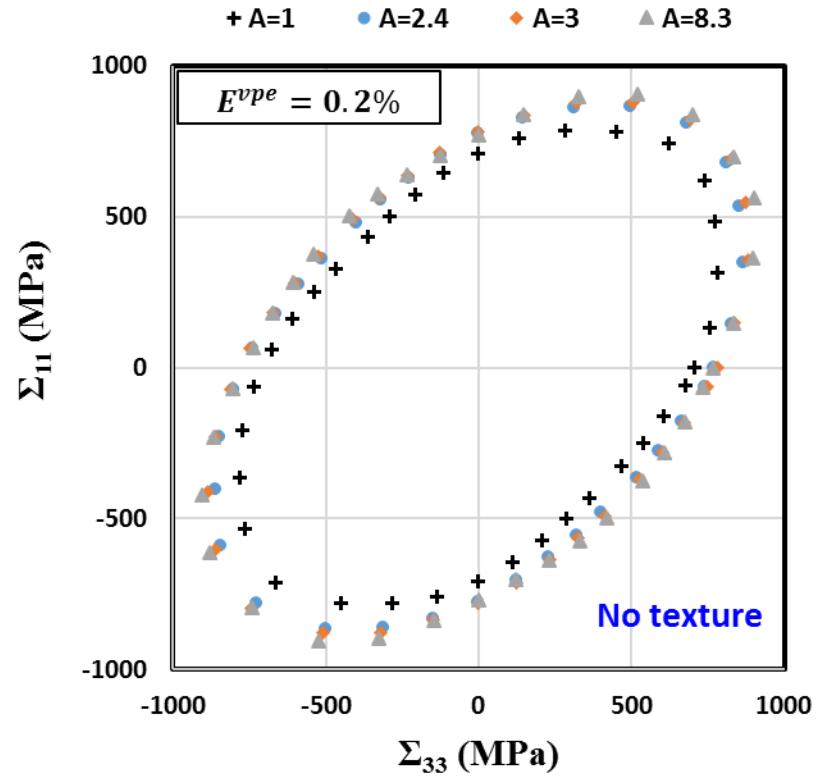
$\{112\} <111>$ slip systems are predominant at the onset of plasticity when elastic anisotropy

Influence of β elastic anisotropy on the Bauschinger stress

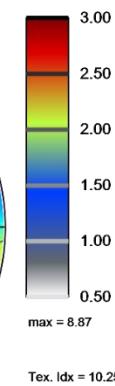
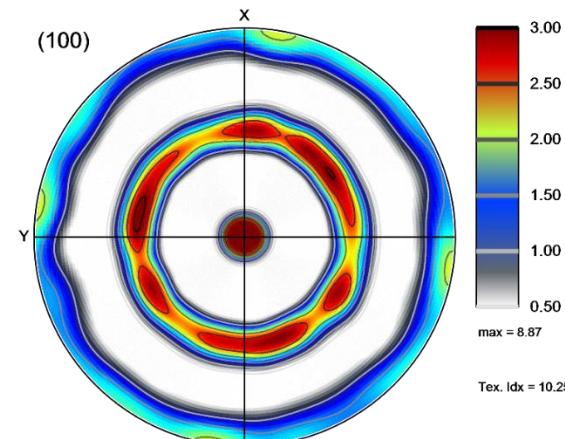
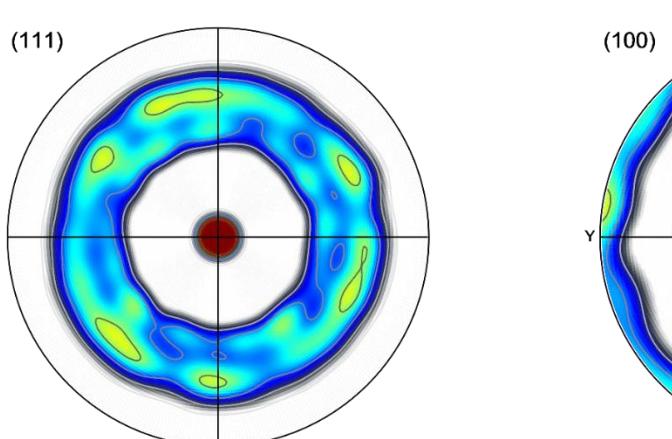
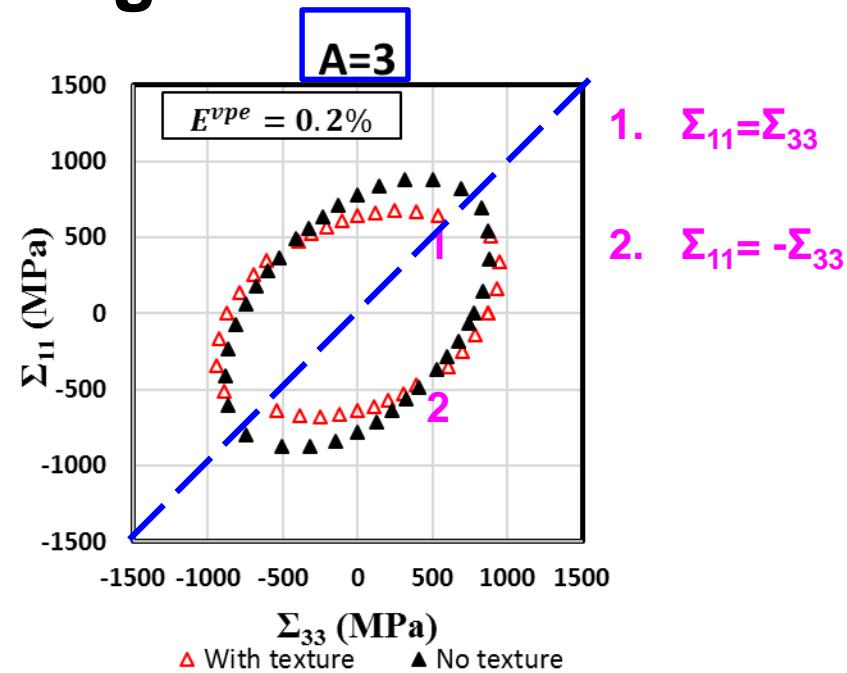
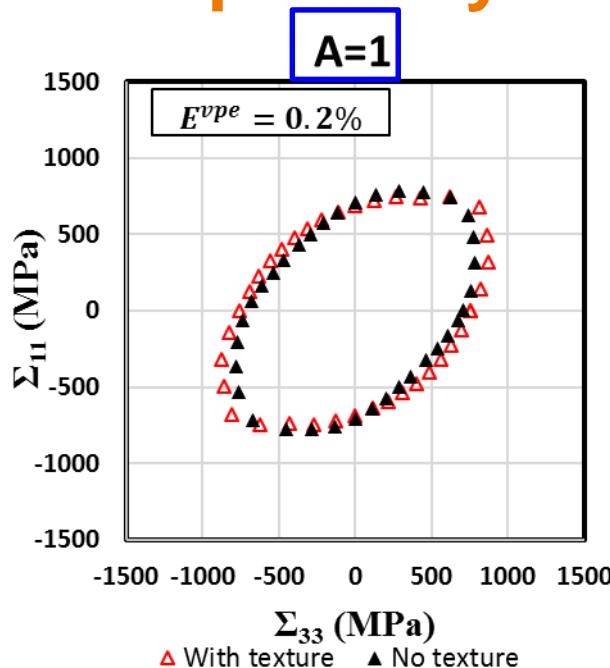
Cyclic tension-compression loading simulations are performed at an applied strain rate of $2 \times 10^{-3} s^{-1}$ with strain amplitude of $-/+ 5\%$



Influence of elastic anisotropy on the multiaxial plastic yielding- random texture



Influence of elastic anisotropy on the multiaxial plastic yielding- β -forged texture



Tex. idx = 10.25

Stereographic (111) and (100) pole figures illustrating the β -forged crystallographic texture. The Texture Index measuring the degree of anisotropy of the texture (Bunge, 1982) is 10.25. These pole figures were generated using the ATEX-software (Beausir and Fundenberger, 2018).

Outline

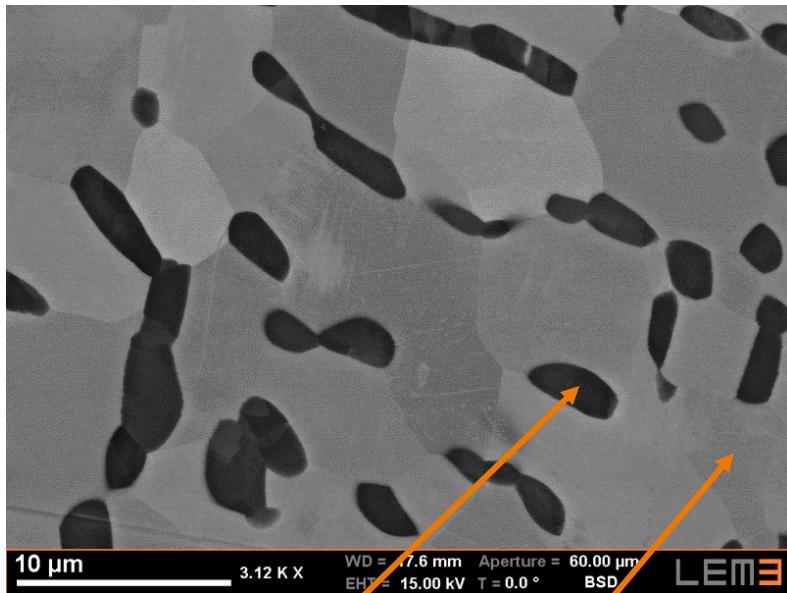
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Nodular microstructure of Ti-1023

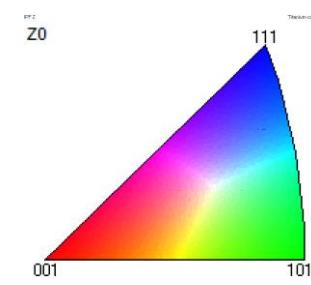
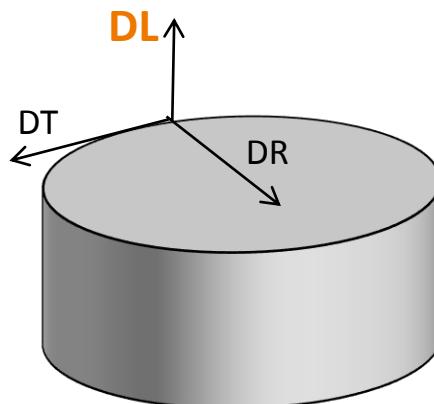
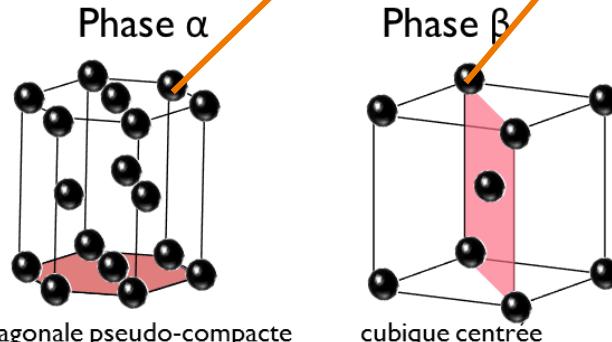
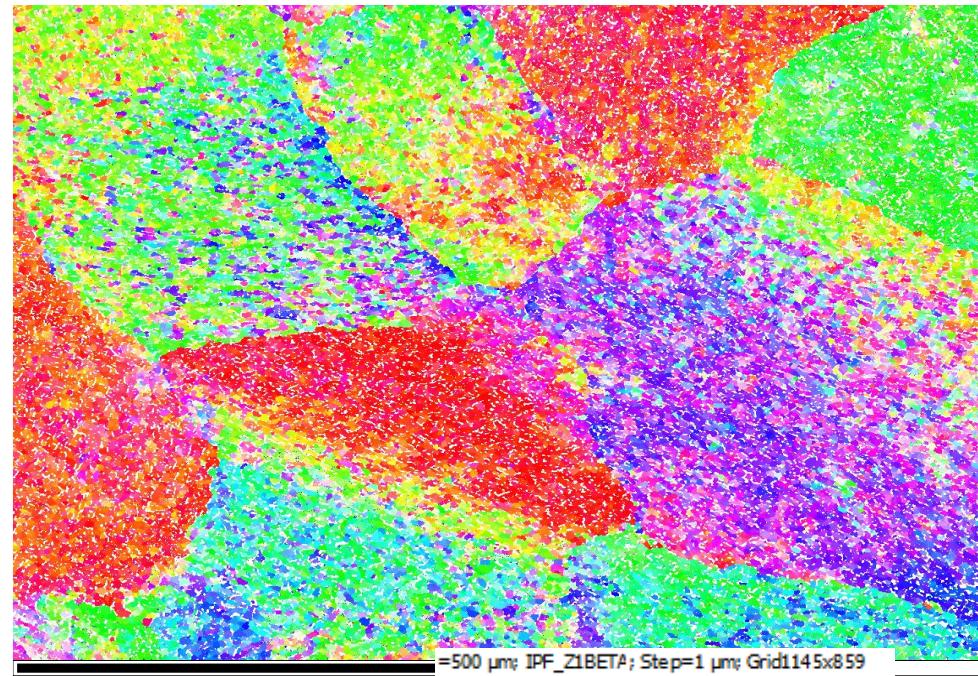
Nodular Microstructure

(13-14% Nodules + 87% β -phase quantified by X-ray Diffraction (O. Perroud))

Random texture



Millimeter large prior β grains

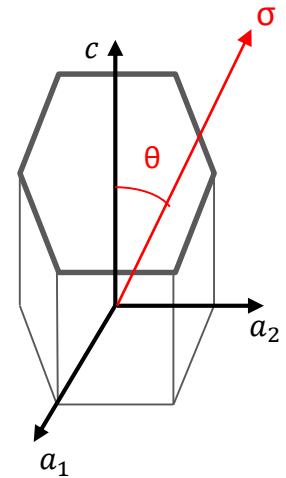
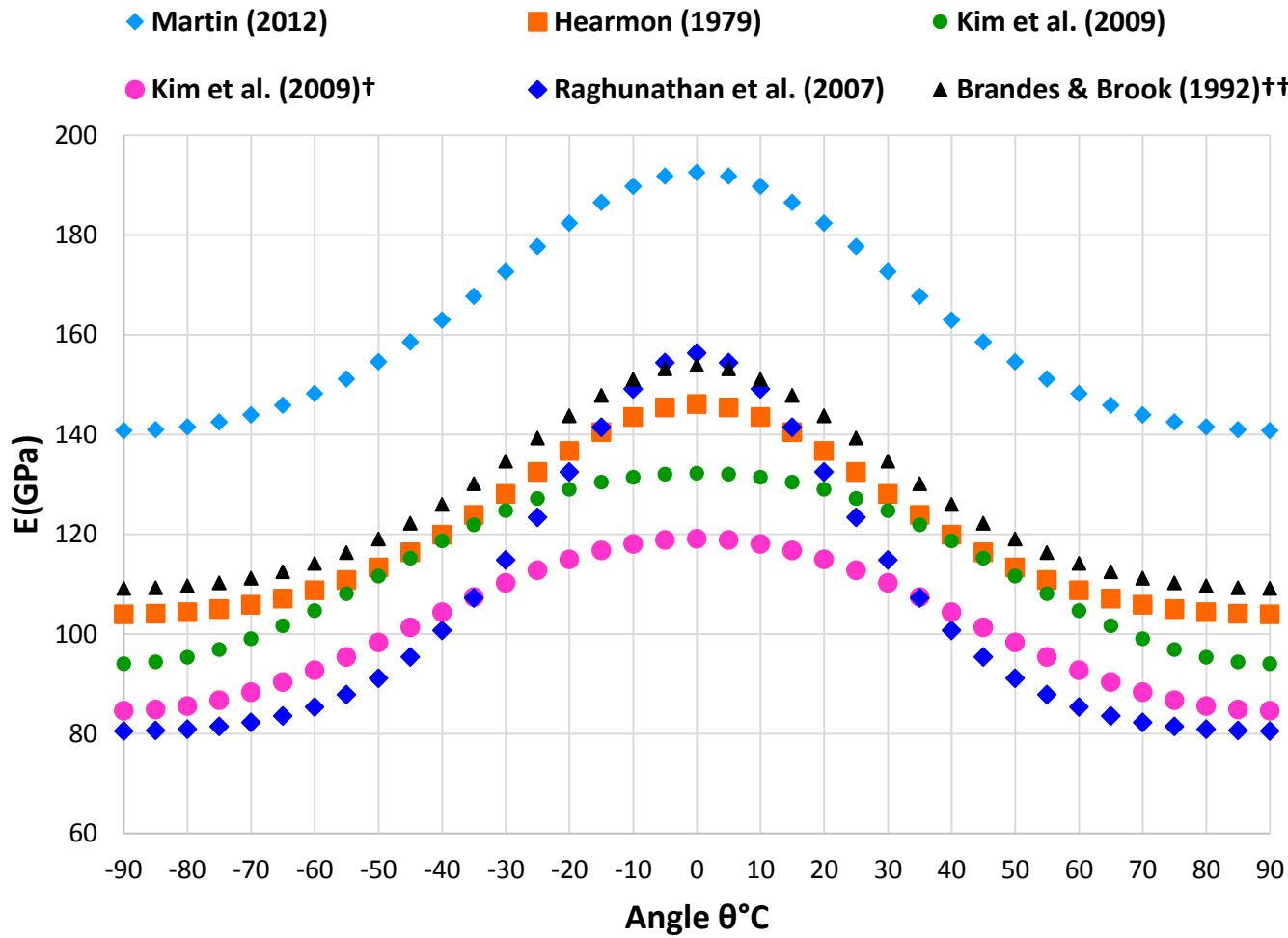


Selection from the literature of EC of the α -phase

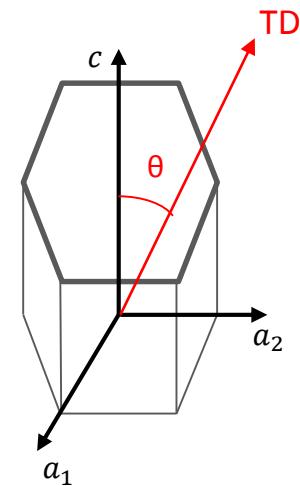
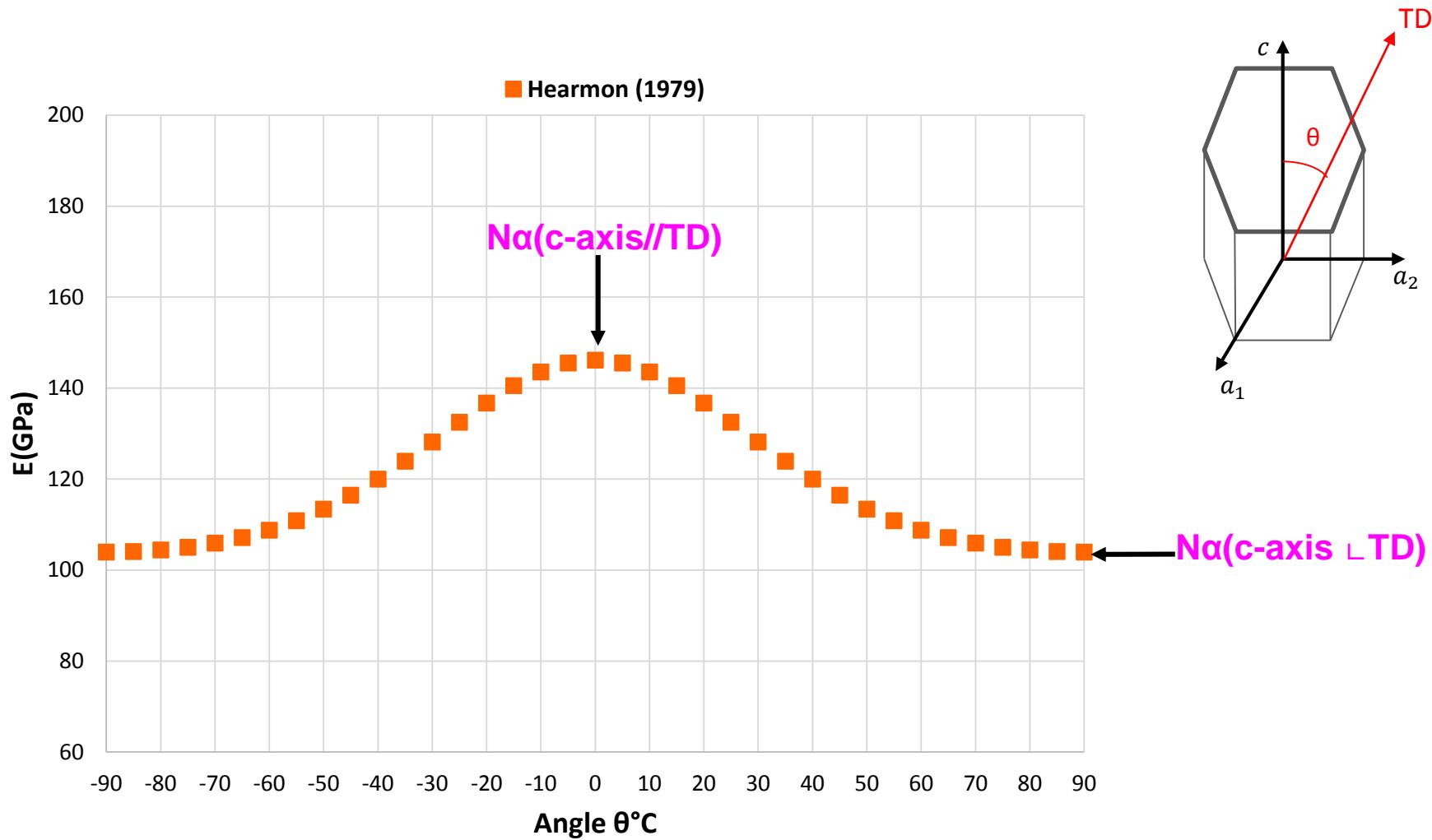
Author	C11	C33	C44	C12	C13	Material	Anisotropy coef. (A)
Hearmon (1979)	160	181	46.5	90	66	Pure α single crystal	0.917562724
Kim et al. (2009)	141	163	48.7	76.9	57.9	α/β single colony Ti-6242	1.026159334
Kim et al. (2009)†	136	163	40.6	78	68.5	A single crystal Ti-6%Al	1.001818182
Fisher et al. (1964)	162	180	46.7	92	69	Pure α single crystal	0.937226277
Martin (2012)	219	243	63.5	124	93	Ti-17	0.940700809
Brandes et Brook, 1992	160	181	46.5	90	66	Pure α single crystal	0.917562724
Simmons & Wang, 1971	162	180	47	92	69	??	0.937226277
Brandes et Brook, 1992††	168	190.5	48.8	94.5	69.3	??	0.915814588
Raghunathan et al. (2007)	163	191	38	114	69.3	Ti-10-2-3	0.7602118
deWit(2008)	162.4	180.7	46.7	92	69	Pure α single crystal	0.933575318

$$A = \frac{2 \times (C_{44} + C_{55} + C_{66})}{C_{11} + C_{22} + C_{33} - C_{12} - C_{13} - C_{23}}$$

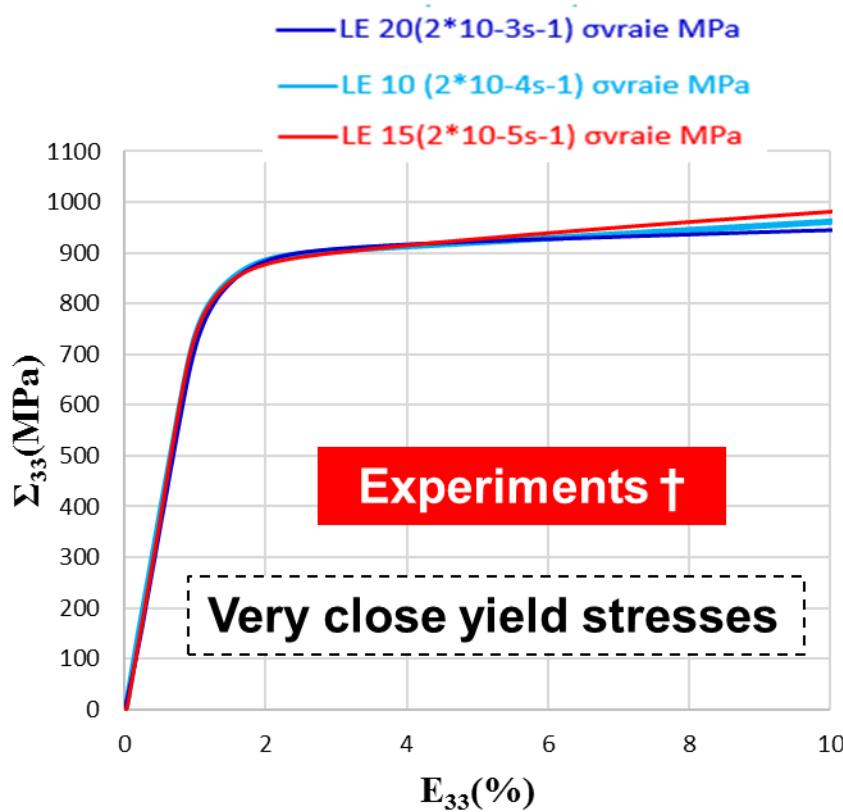
Young modulus of α -single crystal in function of angle θ



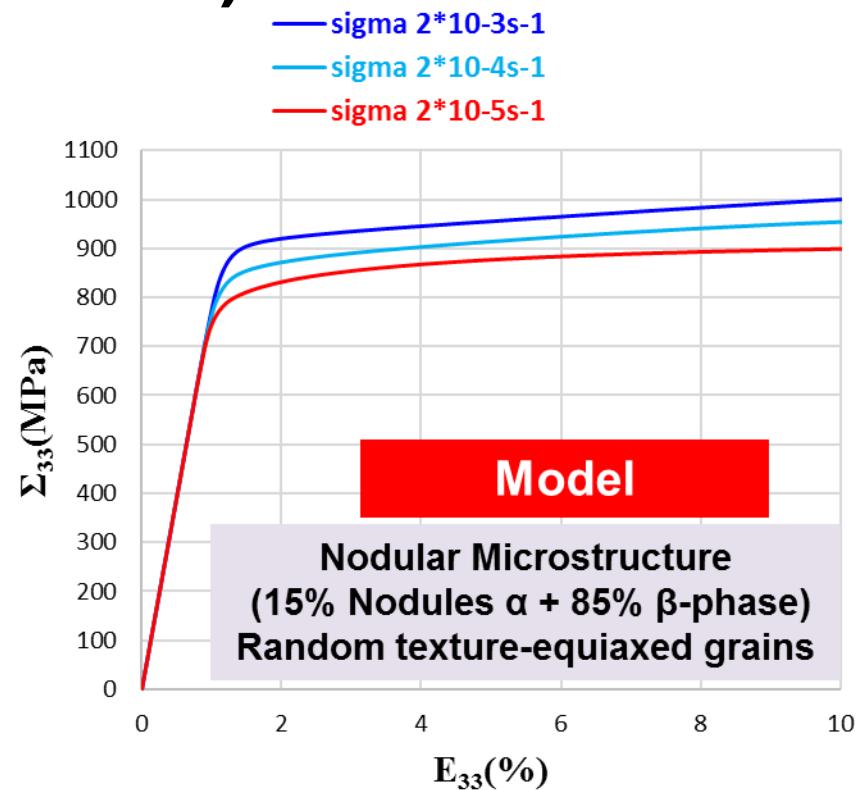
Elastic constants of α -single crystal used in the model



Macroscopic tensile behavior of Ti-1023 (nodular microstructure)



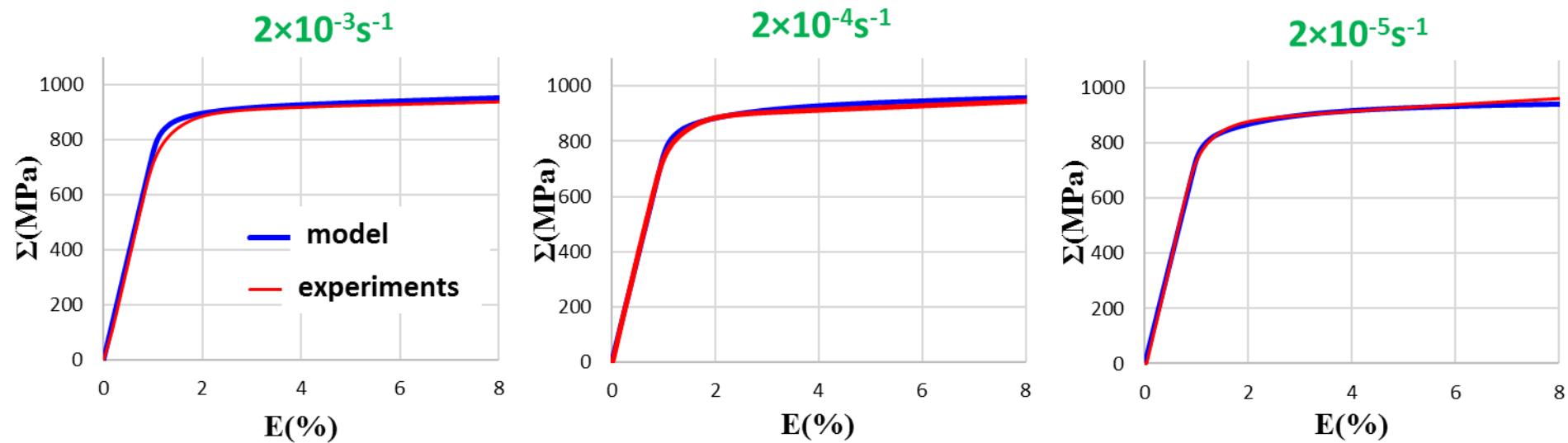
Dimensions : L=20mm ; D= 6mm



β-Phase

slip family	n	σ_0 (MPa)	c^s (MPa)
{110}	20	300	113
{112}	20	300	113
{123}	20	23	400

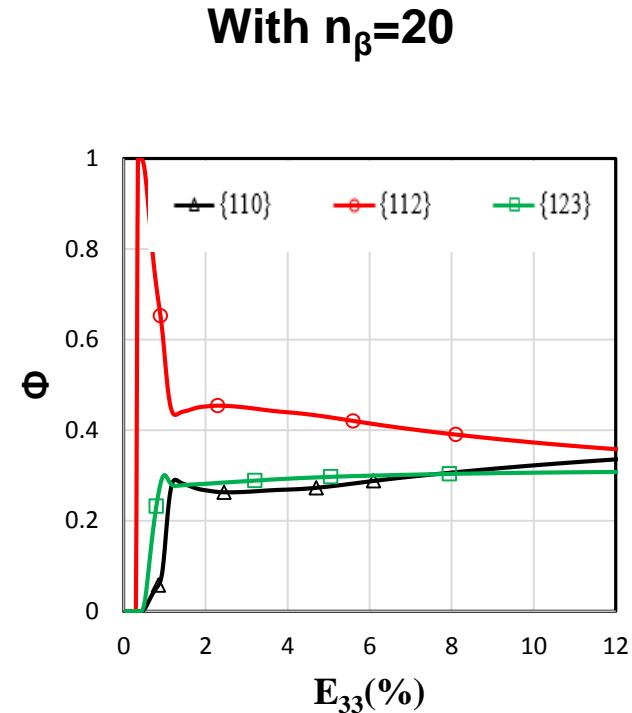
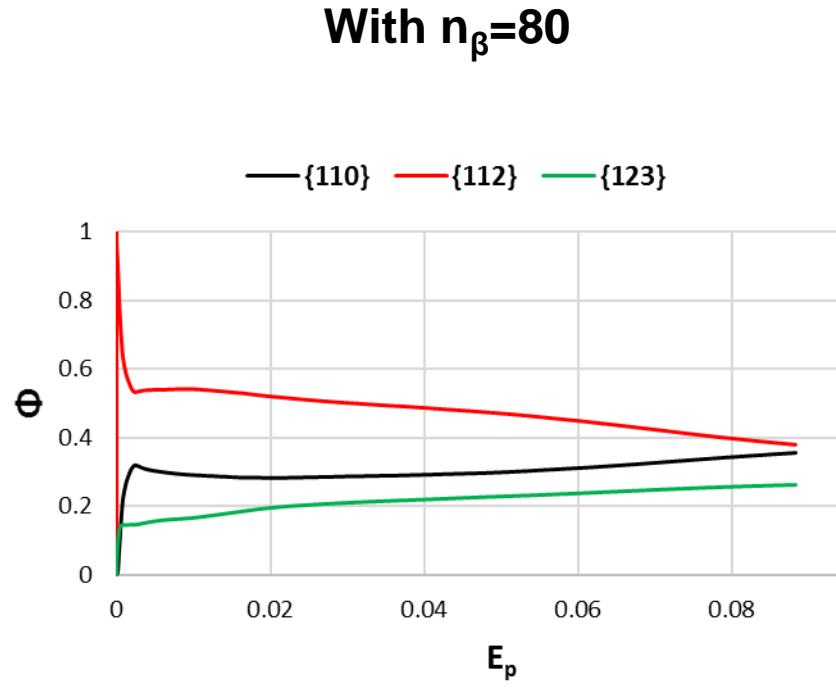
Effect of n_β on the macroscopic tensile behavior of Ti-1023



Slip family	n	$K(\text{MPa} \cdot \text{s}^{1/n})$	$r_0^s(\text{MPa})$	$c^s(\text{MPa})$	Slip family	n	$K(\text{MPa} \cdot \text{s}^{1/n})$	$r_0^s(\text{MPa})$	$c^s(\text{MPa})$
Basal	90	270	215†	0	{110}	80	300	70	200
Prismatic	90	270	350	0	{112}	80	300	70	200
Pyramidal $\langle a \rangle$	90	270	435	0	{123}	80	300	80	400
Pyramidal $\langle c+a \rangle$	90	270	620	0					

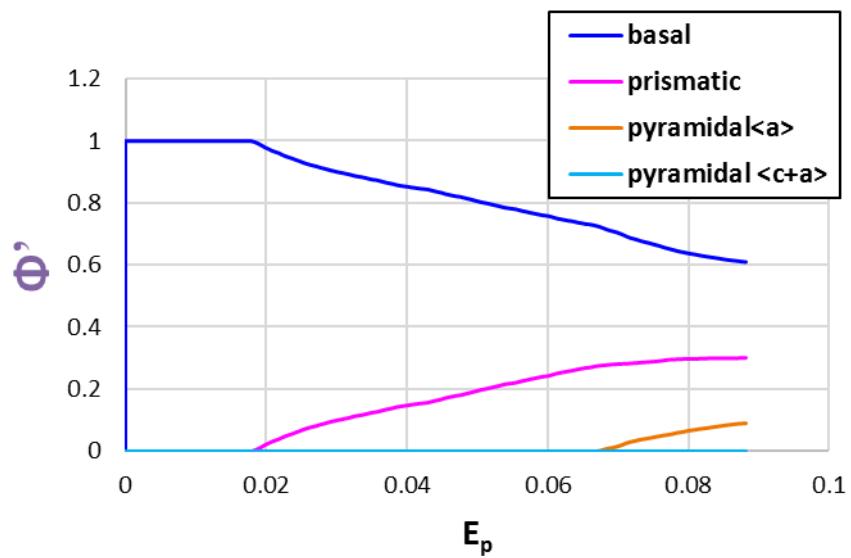
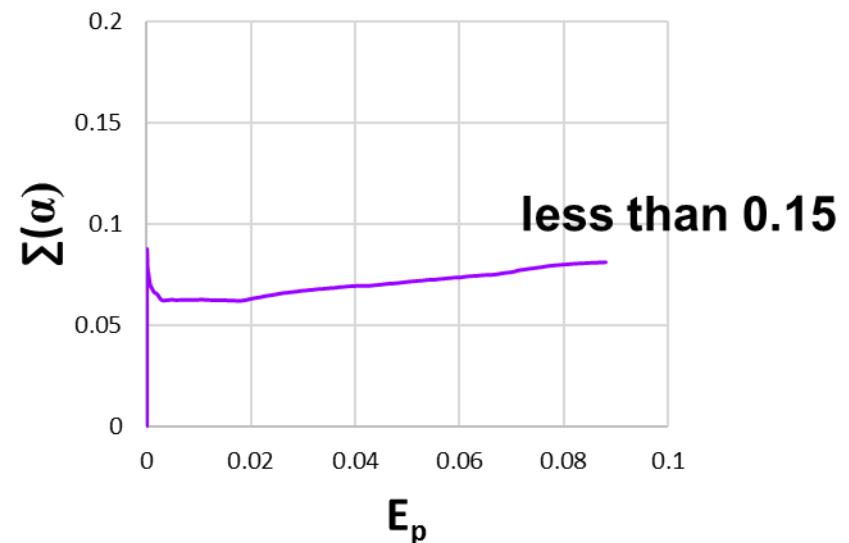
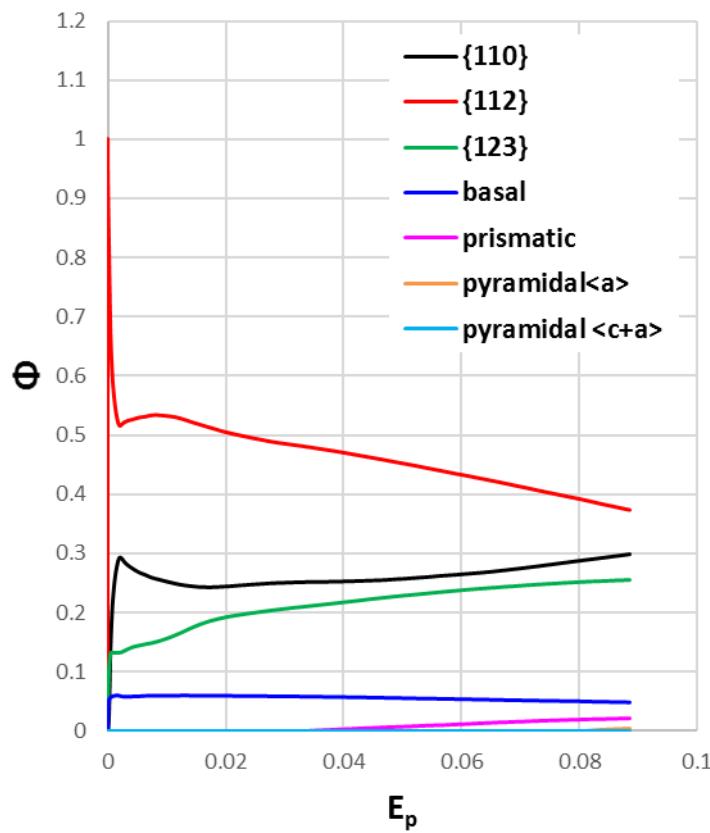
† Based on observations of T. Duval (PhD Thesis, ENSMA, 2013)

Effect of n_{β} on the slip activity for a fully β -equiaxed microstructure



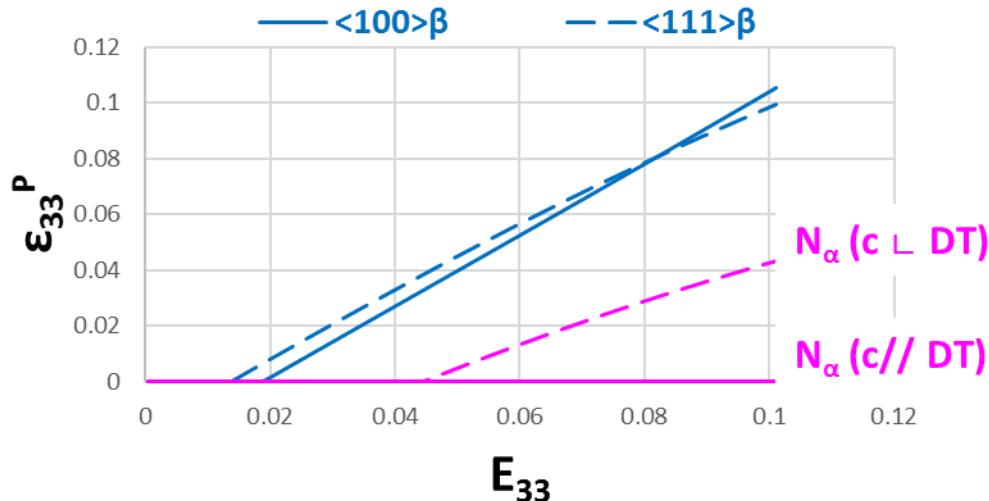
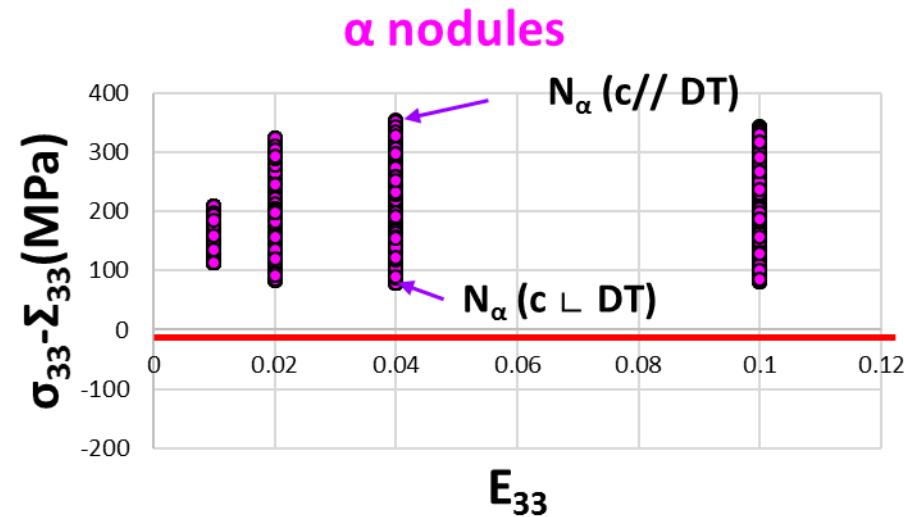
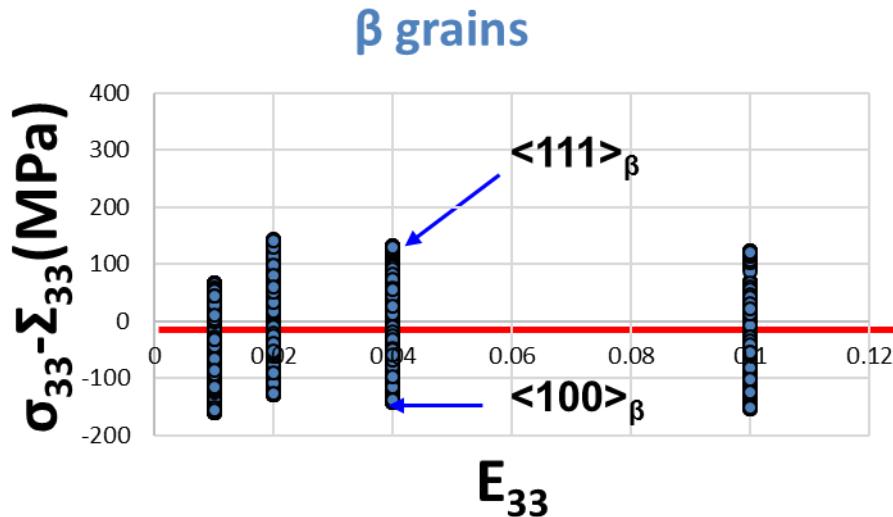
When n_{β} increases, {123} slip family becomes less of priority

Slip activity of Ti-1023 (nodular micro. with 15% α)



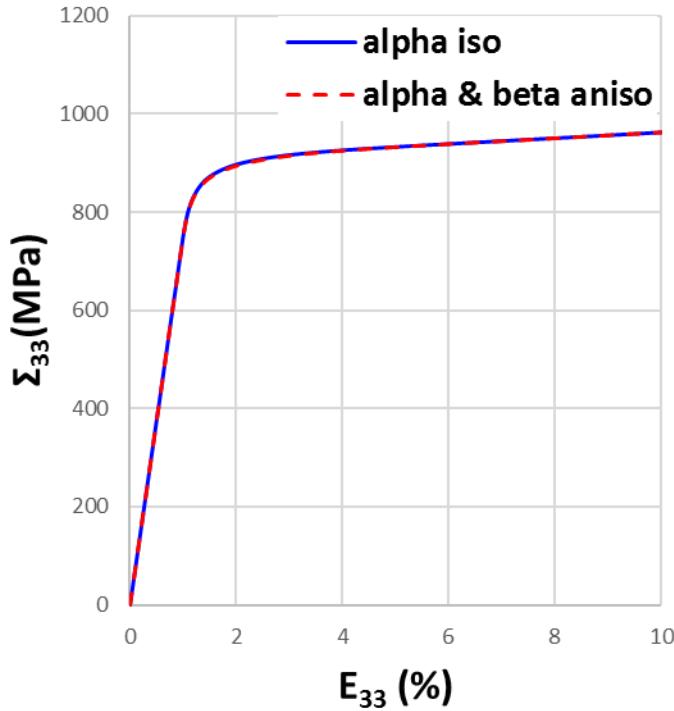
$$\Phi' = \frac{\sum_{g=1}^{ng} \sum_{s=p}^q f_g |\dot{\gamma}_g^s|}{\sum_{g=1}^{n\alpha} \sum_{s=1}^{ns} f_g |\dot{\gamma}_g^s|}$$

Plastic strain in α nodules (c//TD and c \perp TD)

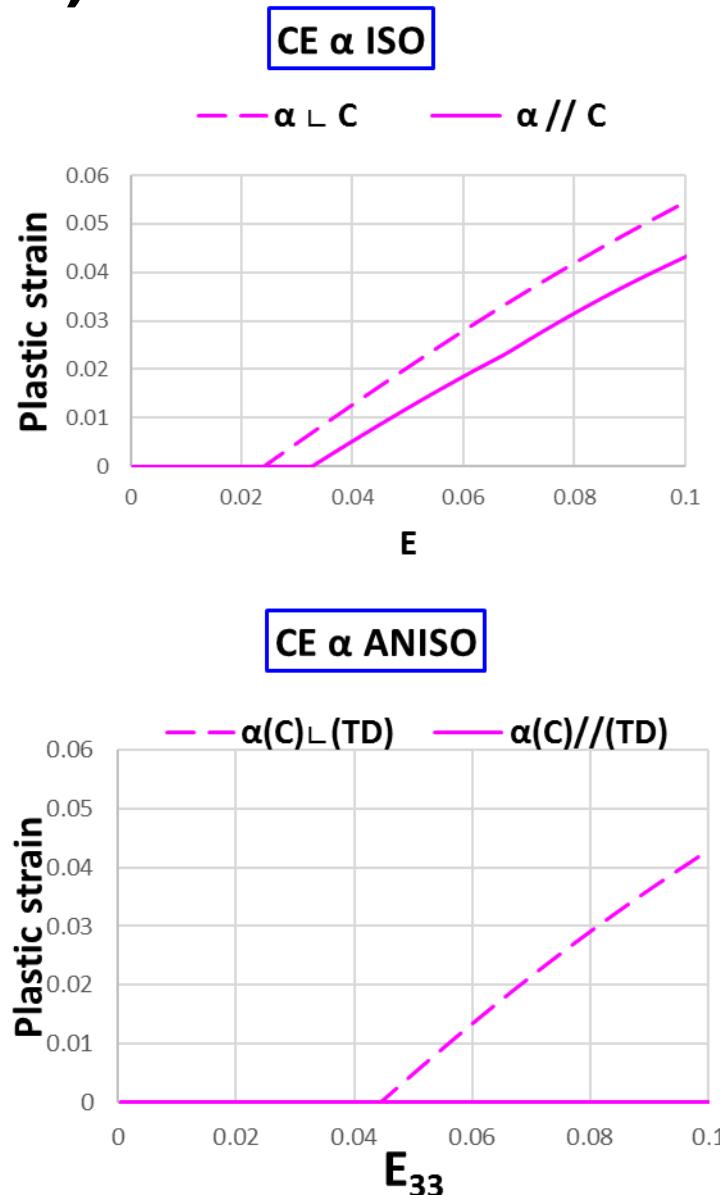


Slip family	r_0^s (MPa)
Basal	215
Prismatic	350
Pyramidal $\langle a \rangle$	435
Pyramidal $\langle c+a \rangle$	620

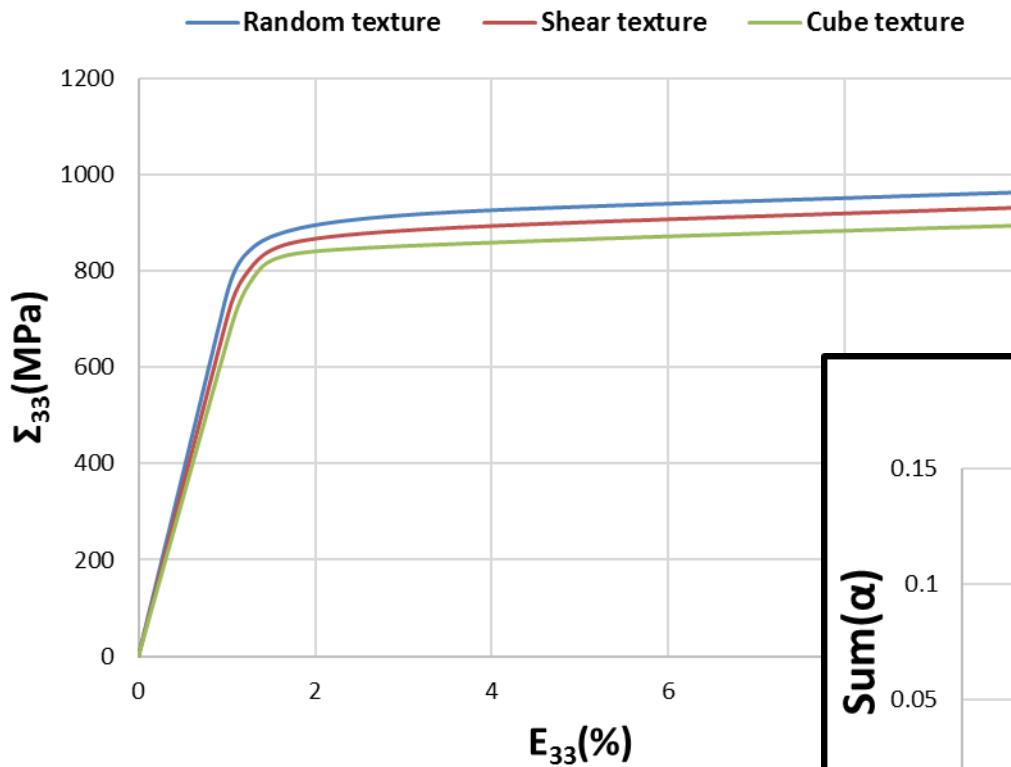
α -phase anisotropic elasticity VS isotropic elasticity (A=1)



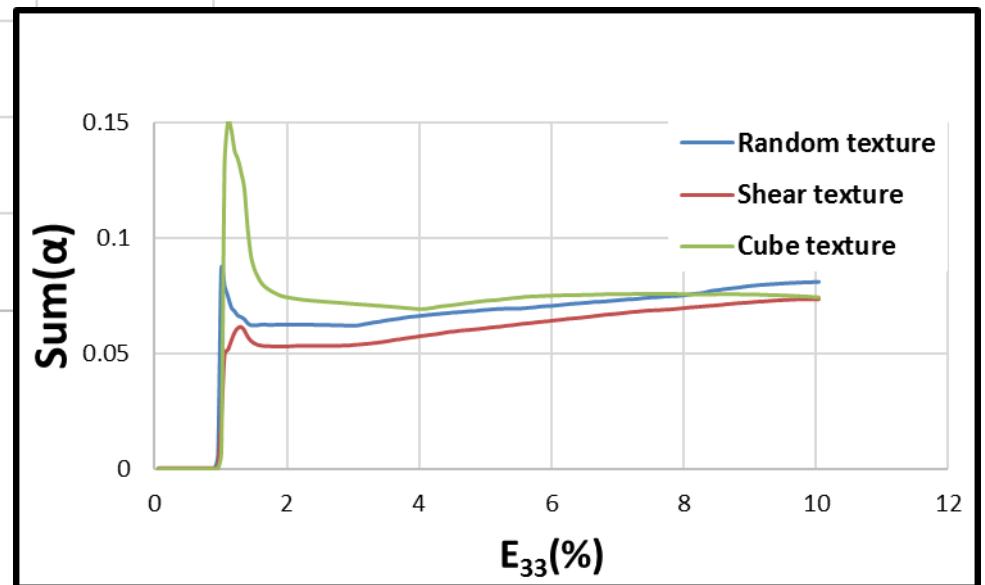
Nodular Microstructure
(15% Nodules α + 85% β -phase)
Random texture-equiaxed grains



Influence of texture on the slip activity of α -phase



**Nodular Microstructure
(15% Nodules α + 85% β -phase)
equiaxed grains**



Cube texture is favorable to α -phase slip activity

Conclusions

An advanced micromechanical model (EVPSC) is applied to near β -Ti alloys:

- Macroscopic behavior is not discriminant to evaluate the effect of the β elastic anisotropy.
- Influence of elastic anisotropy (A) on incompatibility stresses: different local behaviors between $<100>_{\beta}$ and $<111>_{\beta} // TD$.
- Incompatibility stresses of all α nodules are positive no matter what orientation has the nodule/TD.
- α nodules with axis \vec{c}/TD : orientation is unfavorable to activation of slip systems.
- Cube texture is favorable to α -phase slip activity.

Prospects of this work

Consolidate the model results through an experimental campaign

- Evaluate slip activity of α nodules by microscopy coupled to EBSD
- Measure stress by phase field (in situ characterization, synchrotron) : Postdoc Ravi,
start in March 2019 (IRT funding)

Une liste des papiers/communications avec remerciements au Labex 2017-2019

- 1) **Lhadi S.**, Berbenni S., Gey N., Richeton T., Germain L., 2019. Strain rate sensitive behavior and slip activity of Ti 10-2-3 beta-metastable alloy: experiments and micromechanical modeling. Acta Materialia –in preparation-.
- 2) **Lhadi S.**, Berbenni S., Gey N., Richeton T., Germain L., 2018. Micromechanical modeling of the effect of elastic and plastic anisotropies on the mechanical behavior of β -Ti alloys. International Journal of Plasticity. 109 (2018) 88-107.
- 3) **Lhadi S.**, Berbenni S., Richeton T., Gey N., Germain L., 2018. Micromechanical modelling of the elastoviscoplastic behavior and incompatibility stresses of near beta-titanium alloys, 2018. Special Issue Labex DAMAS in Materials MATERIALS 2018, 11(7), 1227.
- 4) **Lhadi S.**, Berbenni S., Gey N., Richeton T., Germain L. Effet de l'anisotropie élastique de la phase β sur le comportement mécanique en traction des alliages de titane β -métastables. Conférence Matériaux à Strasbourg, 19-23 Novembre 2018.
- 5) **Lhadi S.**, Berbenni S., Gey N., Richeton T., Germain L. Effect of elastic anisotropy on the fatigue behavior of near- β titanium alloys thanks to an elasto-viscoplastic self-consistent model. The 12th International Fatigue Congress, May 27th- June 1st, 2018, Poitiers, France.
- 6) **Lhadi S.**, Berbenni S., Gey N., Richeton T., Germain L. An affine elastic-viscoplastic self-consistent model to study incompatibility stresses in near beta-Ti alloys. 5th International Conference on Material Modelling, 13-16 June, 2017, Rome, Italy.

Micromechanical modeling of near β -Ti alloys: Effect of elastic anisotropy on the overall elasto- viscoplastic behavior, incompatibility stresses and slip activity

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