A Multiscale and Thermomechanical Modeling of Shape Memory Alloys using CAST3M

PhD student (Reporter): **Xiaofei JU** (xiaofei.ju@ensta-paris.fr)

Supervisor: **Ziad MOUMNI** (ziad.moumni@ensta-paris.fr)

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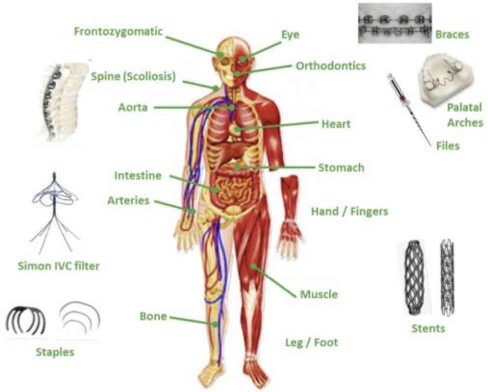
Backgrounds-NiTi Shape Memory Alloys (SMAs)

■ Unique Properties

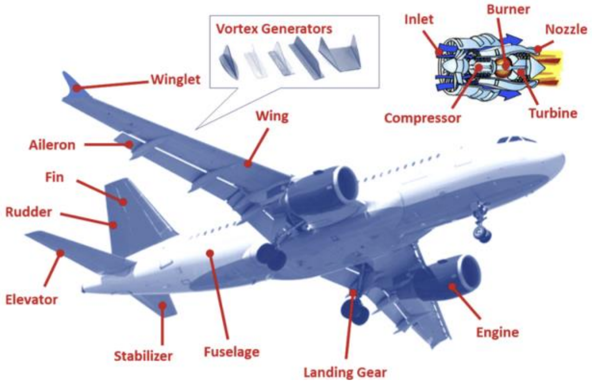
Shape Memory Effect: Recover their shape by simple heating after being inelastically strained

Pseudoelasticity: Accommodate large recoverable inelastic strains (6-8%)

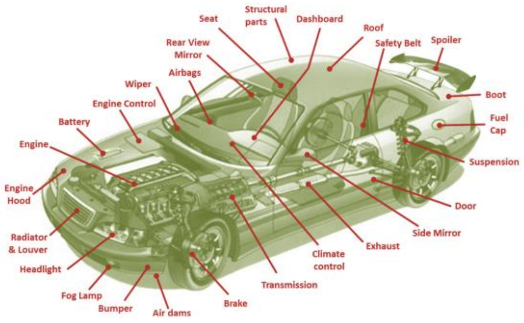
■ Applications



Biomedical



Aerospace



Automotive

Robotic

- **Promising Material** in Applications of Biomedical, Aerospace…
- Safety Problem Related with **Cycle Fatigue Issue**
- A **Micromechanical-based Model** Required for Fatigue Analysis

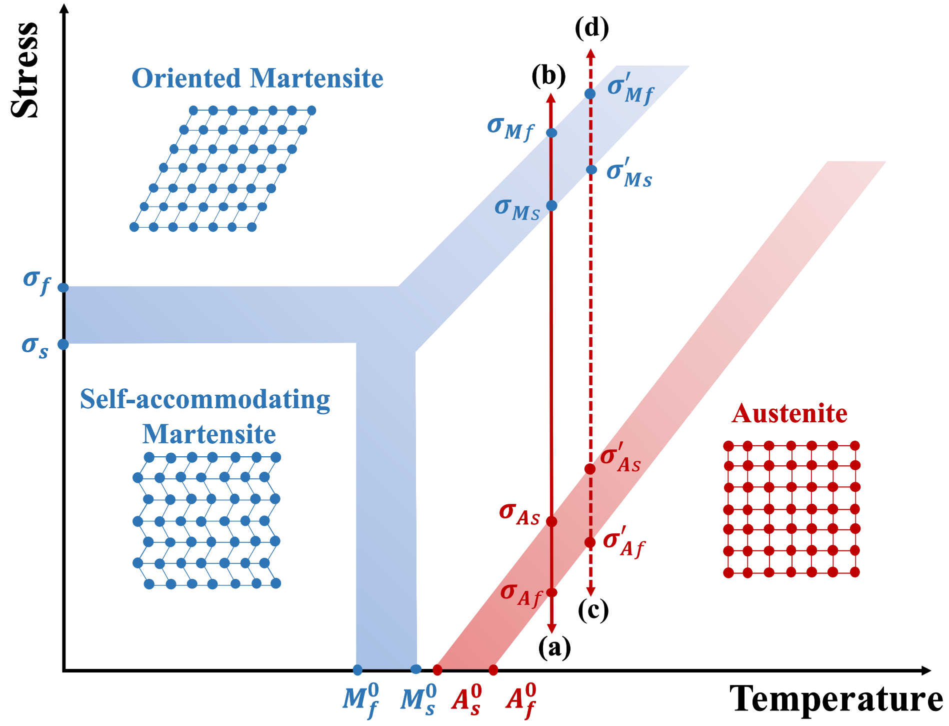
Jani J M, Leary M, Subic A, et al. ,Materials & Design, 2014

Backgrounds – Inelastic Mechanisms

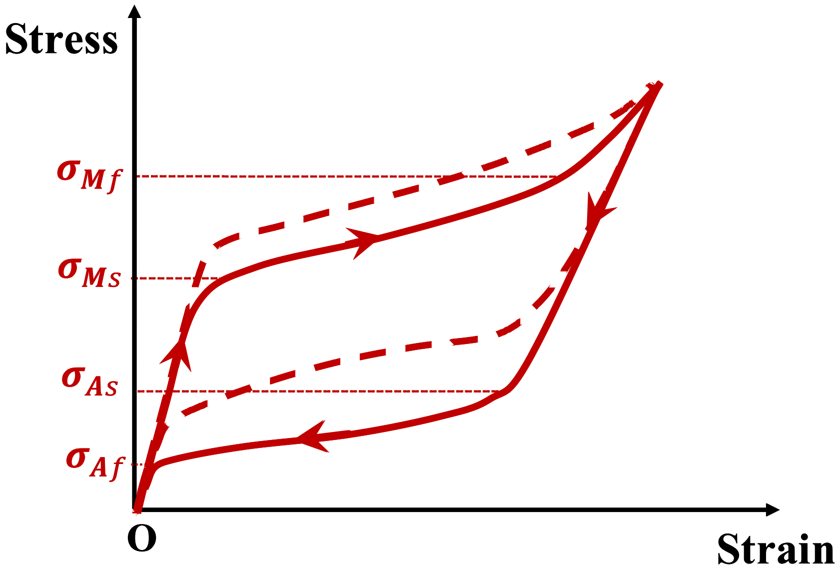
- ## Martensitic Transformation

A solid-solid **phase change** between cubic **austenite** and **martensitic** phase

Pseudoelasticity: T>A_f^0



Mechanical Response

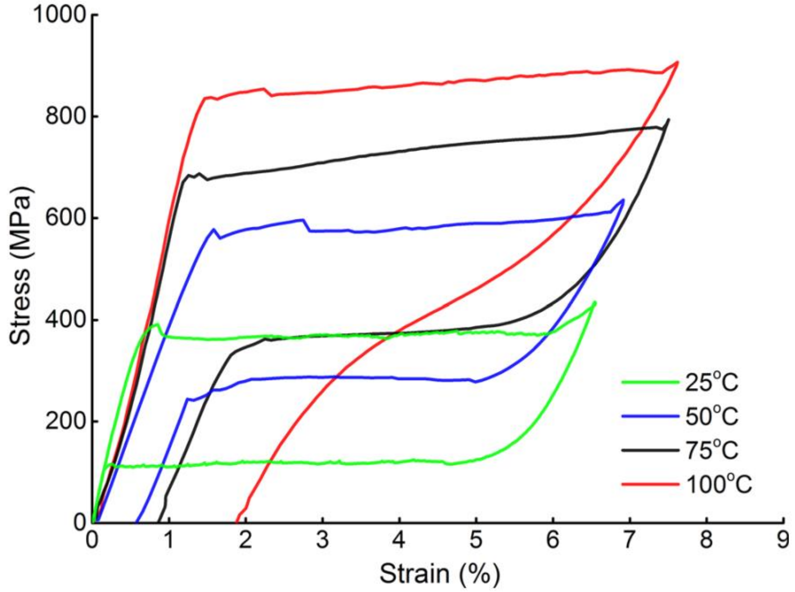


- ## Thermomechanical Coupling Effect

Backgrounds – Inelastic Mechanisms

- **Deformation Slip in Austenite**

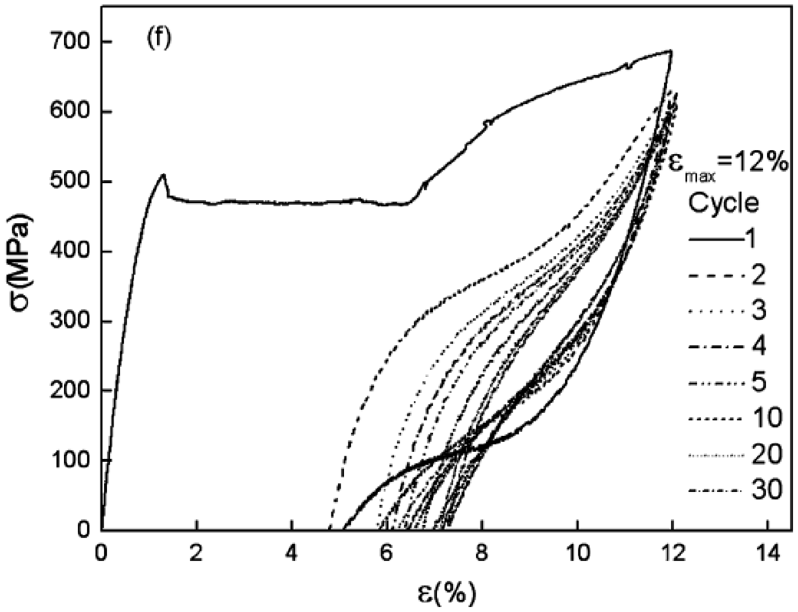
High Temperature



Xiao Y, Zeng P, Lei L, et al. Shape Memory and Superelasticity, 2015

- **Deformation Twinning in Martensite**

Large Strain



Wang X, Xu B, Yue Z. Journal of Alloys and Compounds, 2008

Backgrounds – Inelastic Mechanisms

■ Transformation-induced Plasticity (TRIP)

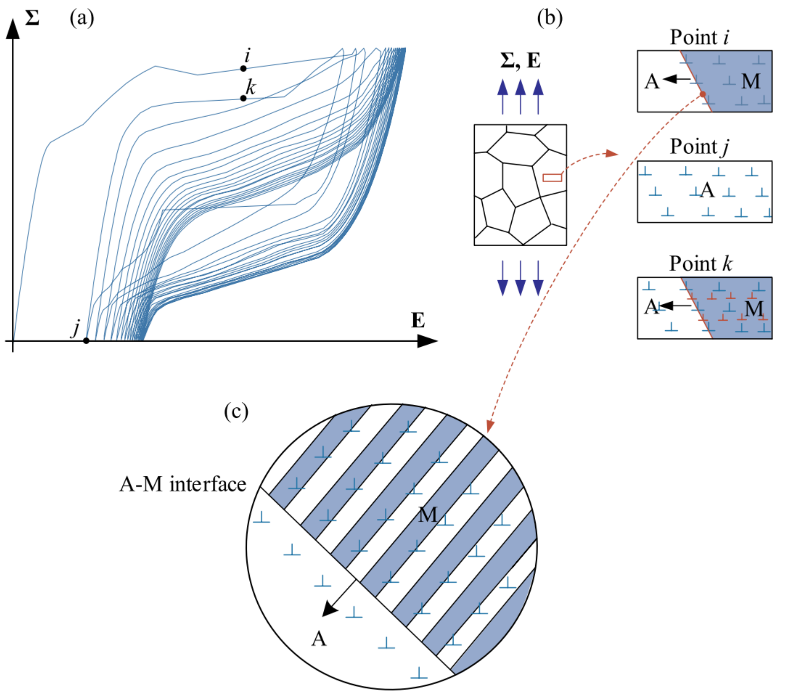


Fig. 1. Schematic of TRIP deformation, Σ and *E* are global stress and strain, A and M represent austenite and martensite phases: (a) macroscopic stress-strain response; (b) the accumulation of dislocations at mesoscopic scale; (c) at microscopic scale, generation of the dislocation slip is located in austenite phase in front of A-M interface in order to achieve compatibility (Paranjape et al., 2017; Sittner et al., 2018; Heller et al., 2018).

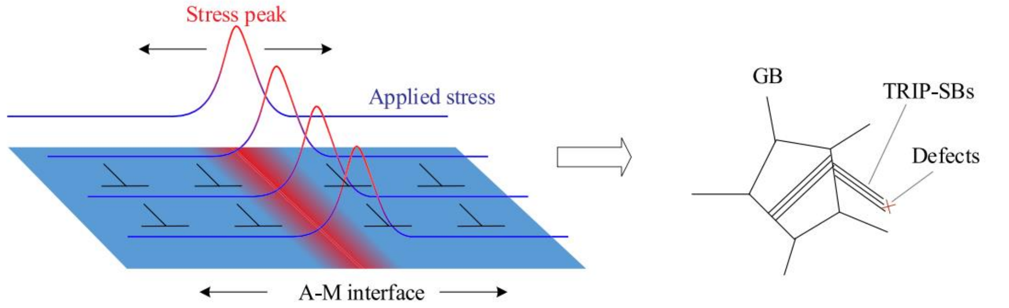


Fig. 2. Schematic of stress peak in A-M interface initiating fatigue cracks through interactions between TRIP-SBs and grain boundary (GB), or other defects inside the material.

Zhang Y, Moumni Z, You Y, et al. International Journal of Plasticity, 2019

Motivations - Originality

Table 1
Summary of micromechanical constitutive models.

Models	Features Finite strain theory	A	B	C	D	E	F
Thamburaja and Anand (2001)	✓	✓					
Lim and McDowell (2002)		✓				✓	
Anand and Gurtin (2003)	✓	✓				✓	
Thamburaja (2005)	✓	✓					
Wang et al. (2008b)		✓		✓			
Manchiraju and Anderson (2010)	✓	✓	✓				
Richards et al. (2013)		✓	✓				✓
Mirzaeifar et al. (2013)		✓				✓	
Yu et al. (2013, 2015c)		✓			✓		✓
Yu et al. (2014a)		✓	✓	✓			✓
Yu et al. (2014b)		✓			✓		✓
Yu et al. (2014c)		✓			✓	✓	✓
Yu et al. (2015a)		✓	✓		✓		✓
Paranjape et al. (2016)	✓	✓	✓				
Xiao et al. (2018)		✓			✓	✓	✓
Paranjape et al. (2018)	✓	✓					
Yu et al. (2018)		✓				✓	
Dhala et al. (2019)	✓	✓	✓	✓			
Xie et al. (2019)		✓	✓		✓		✓
Xie et al. (2020)		✓	✓		✓	✓	✓
Ebrahimi et al. (2020)		✓			✓		✓
Hossain and Baxevanis (2021)	✓	✓	✓		✓	✓	
Xu et al. (2021)		✓	✓	✓	✓	✓	✓
Present work	✓	✓	✓	✓	✓	✓	✓

Notes: A: phase transformation; B: deformation slip in austenite; C: deformation twinning in martensite; D: TRIP; E: thermomechanical coupling effect; F: cyclic loading (cycling up to the shakedown (stabilized) state).

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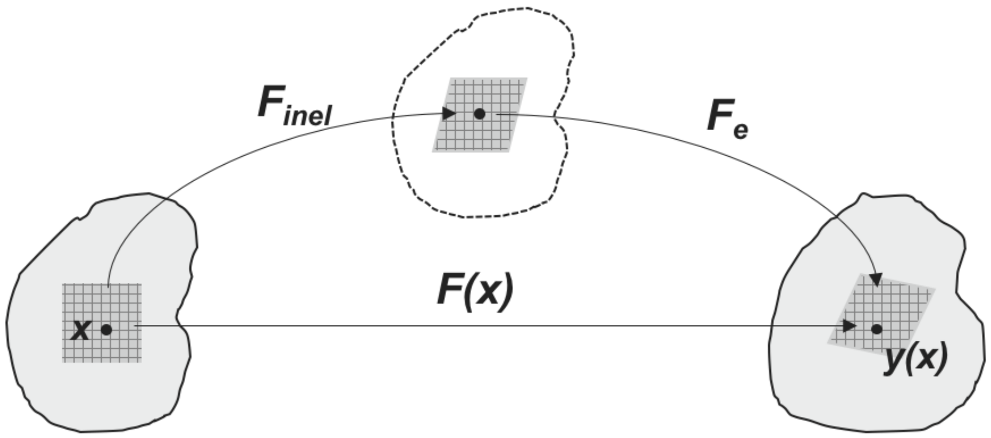
Constitutive Equations

Main Equations



- **Deformation Gradient $\boldsymbol{F}$**

$$\boldsymbol{F} = \boldsymbol{F}_e \boldsymbol{F}_{inel}$$

- **Elastic Green Strain $\boldsymbol{E}_e$**

$$\boldsymbol{E}_e = \frac{1}{2}(\boldsymbol{U}_e{}^2 - \boldsymbol{I}) \text{ while } \boldsymbol{F}_e = \boldsymbol{R}_e \boldsymbol{U}_e$$

- **Hooke's Law**

$$\boldsymbol{T} = \mathbb{C} : \boldsymbol{E}_e$$

- **Cauchy Stress $\boldsymbol{\sigma}$**

$$\boldsymbol{\sigma} = \frac{1}{det(\boldsymbol{F}_e)} \boldsymbol{F}_e \boldsymbol{T} \boldsymbol{F}_e^T$$

- **Velocity Gradient $\boldsymbol{L}$**

$$\boldsymbol{L} = \dot{\boldsymbol{F}} \boldsymbol{F}^{-1} = \boldsymbol{L}_e + \boldsymbol{F}_e \boldsymbol{L}_{inel} \, \boldsymbol{F}_e{}^{-1}$$

- **Inelastic Part of $\boldsymbol{L}$**

$$\boldsymbol{L}_{inel} \approx \boldsymbol{L}_p^A + \boldsymbol{L}_{tr} + \boldsymbol{L}_{trip} + \boldsymbol{L}_p^M$$

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Constitutive Equations

Main Equations

$$L_{inel} \approx L_p^A + L_{tr} + L_{trip} + L_p^M$$

- $L_p^A = (1-\xi)\sum_{\alpha=1}^{24} \dot{\gamma}_A^{(\alpha)} S_p{}^{(\alpha)}$
- $L_{tr} = \sum_{i=1}^{24} \dot{\xi}^{(i)} g_{tr} S_{tr}{}^{(i)}$
- $L_{trip} = (1-\xi)\sum_{\alpha=1}^{24} \dot{\gamma}_{trip}^{(\alpha)} S_p{}^{(\alpha)}$
- $L_p^M = \xi \sum_{t=1}^{11} \dot{\gamma}_{tw}^{(t)} S_{tw}{}^{(t)}$

- **Orientation Tensor**

$$S_p{}^{(\alpha)} = m_0{}^{(\alpha)} \otimes n_0{}^{(\alpha)}$$

$$S_{tr}{}^{(i)} = b_0{}^{(i)} \otimes d_0{}^{(i)}$$

$$S_{tw}{}^{(t)} = b_0^{tw(t)} \otimes d_0^{tw(t)}$$

State Variables

$$E_e,\ \xi^{(i)},\theta,\ \dot{\gamma}_A^{(\alpha)},\ \dot{\gamma}_{tw}^{(t)},\ \dot{\gamma}_{trip}^{(\alpha)},\ B_{int}$$

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Constitutive relations

- **Helmholtz free energy density**

$$\psi\left(\boldsymbol{E}_e, \xi^{(i)}, \theta\right) = \psi_e + \psi_\theta + \psi_{int} + \psi_p + \psi_{trans} + \psi_{cst}$$

where,

$$\psi_e = \frac{1}{2}\boldsymbol{E}_e : \mathbb{C} : \boldsymbol{E}_e$$

$$\psi_\theta = C\left[(\theta - \theta_0) - \theta \ln\frac{\theta}{\theta_0}\right] + \mu(\theta - \theta_0)\xi$$

$$\dot{\psi}_{int} = -\boldsymbol{B}_{int} : \left(\boldsymbol{L}_{tr} + \boldsymbol{L}_{trip}\right)$$

$$\dot{\psi}_p = (1-\xi)\sum_{\alpha=1}^{24} g_A^{(\alpha)}\left|\dot{\gamma}_A^{(\alpha)}\right| + \xi\sum_{t=1}^{11} g_{tw}^{(t)}\left(\dot{\gamma}_{tw}^{(t)}\right)$$

$$\psi_{trans} = \frac{1}{2}G\xi^2 + \frac{1}{2}\beta g_{tr}\xi(1-\xi)$$

$$\psi_{cst} = -w_0(1-\xi) - \sum_{i=1}^{N_T} w_i \xi^{(i)}$$

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Constitutive relations

- **Evolution laws**

  - **Plasticity in austenite**

$$\dot{\gamma}_A^{(\alpha)} = \dot{\gamma}_A^0 \left|\frac{\tau_A^{(\alpha)}}{g_A^{(\alpha)}}\right|^{\frac{1}{m_A}} \operatorname{sign}\left(\tau_A^{(\alpha)}\right), and \;\; \tau_A^{(\alpha)} = \boldsymbol{M}: \boldsymbol{S}_p^{(\alpha)}$$

$$\dot{g}_A^{(\alpha)} = \sum_{\beta=1}^{24} h_A^{\alpha\beta} \left|\dot{\gamma}_A^{(\beta)}\right|$$

  - **Plasticity in martensite**

$$\dot{\gamma}_{tw}^{(t)} = \begin{cases} \dot{\gamma}_{tw}^0 \left(\frac{\tau_{tw}^{(t)}}{g_{tw}^{(t)}}\right)^{\frac{1}{m_{tw}}}, & \tau_{tw}^{(t)} > 0 \\ 0, & \tau_{tw}^{(t)} \leq 0 \end{cases}, and \; \tau_{tw}^{(t)} = \boldsymbol{M}: \boldsymbol{S}_{tw}^{(t)}$$

$$\dot{g}_{tw}^{(t)} = \sum_{s=1}^{11} h_{tw}^{ts} \dot{\gamma}_{tw}^{(s)}$$

  - **Transformation induced plasticity (TRIP)**

$$\dot{\gamma}_{trip}^{(\alpha)} = \begin{cases} \frac{\gamma_{sat}}{b_1} e^{-\frac{\xi c}{b_1}} |\dot{\xi}| \operatorname{sign}\left(f_{trip}^{(\alpha)}\right) & \text{when } SF_{plastic}^{(\alpha)} > SF_{critical} \\ 0 & \text{otherwise} \end{cases}$$

  - **Transformation**

    - Transformation criteria

$\mathcal{F}_{AM}^{(i)} = f_{tr}^{(i)} - f_c^{(i)} = 0$ Forward transformation

$\mathcal{F}_{MA}^{(i)} = f_{tr}^{(i)} + f_c^{(i)} = 0$ Reverse transformation

    - Consistency conditions

$\mathcal{F}_{AM}^{(i)} = 0 \; and \; \dot{\mathcal{F}}_{AM}^{(i)} = 0 \Rightarrow \dot{\xi} > 0$ Forward transformation

$\mathcal{F}_{MA}^{(i)} = 0 \; and \; \dot{\mathcal{F}}_{MA}^{(i)} = 0 \Rightarrow \dot{\xi} < 0$ Reverse transformation

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Constitutive relations

- **Evolution laws**
  - **Internal variables related with cyclic degradation**

$$\dot{\xi}_{ua}^{(i)} = \frac{\xi_{ua}^{sat}}{b_3} e^{-\frac{\xi_c}{b_3}} \left|\dot{\xi}^{(i)}\right| \qquad \dot{\xi}_{rm}^{(i)} = \frac{\xi_{rm}^{sat}}{b_4} e^{-\frac{\xi_c}{b_4}} \left|\dot{\xi}^{(i)}\right|$$

$$\| \dot{\boldsymbol{B}}_{int}^{(i)} \| = \frac{B_{sat}}{b_2} e^{-\frac{\xi_c}{b_2}} \dot{\xi}_c \qquad \dot{f}_c^{(i)} = \frac{\left(f_{c\_sat}^{(i)} - f_{c\_0}^{(i)}\right)}{b_5} e^{-\frac{\xi_c}{b_5}} |\dot{\xi}| \qquad \dot{G} = \frac{(G^{sat} - G^0)}{b_6} e^{-\frac{\xi_c}{b_6}} |\dot{\xi}|$$

  - **Dislocation density and stored energy**

$$\rho_{tot} = (1-\xi)\rho_A + \xi \cdot \xi_{tw} \cdot \rho_M, \qquad E_{st} \approx \rho_{tot} E_{dis} \approx \frac{1}{2} \rho_{tot} G_{shear} b^2$$

$$\dot{\rho}_A^{(\alpha)} = c_1\left(\sqrt{\sum_{\alpha=1}^{24} \rho_A^{(\alpha)}} - c_2 \rho_A^{(\alpha)}\right)\left(\left|\dot{\gamma}_A^{(\alpha)}\right| + \left|\dot{\gamma}_{trip}^{(\alpha)}\right|\right)$$

$$\dot{\rho}_M^{(t)} = c_3\left(\sqrt{\sum_{t=1}^{11} \rho_M^{(t)}} - c_4 \rho_M^{(t)}\right)\left(\left|\dot{\gamma}_{tw}^{(t)}\right|\right)$$

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Numerical Implementation

Subroutine Interface

```
mo_util = MODE 'MECANIQUE' 'ELASTIQUE' 'ORTHOTROPE' 'NON_LINEAIRE' 'UTILISATEUR' 'NOM_LOI' 'cp'
        'C_MATERIAU' LCMAT ' C_VARINTER' LCVAR ;
```

'C_MATERIAU' – give access to the list of names associated with the material properties, LCMAT

'C_VARINTER' – give access to the list of names associated with the material's internal variables, LCVAR

LCMAT = MOTS 'YG1' 'YG2' 'YG3' 'NU12' 'NU23' 'NU13' 'G12' 'G23' 'G13' 'V1X' 'V1Y' 'V1Z' 'V2X' 'V2Y' 'V2Z'	Demanded by System
'FAI1' 'THTA' 'FAI2'	Euler Angles
'G0' 'G_' 'H0' 'dgam0' 'm' 'a' 'q'	Deformation Slip
'gtr' 'G' 'beta' 'miu' 'theta0' 't_ambient' 'fc'	Transformation
'Gw' 'G_w' 'H0w' 'dxiw' 'mw' 'aw' 'qw'	Deformation twinning
'b_' 'b1' 'b2' 'gam_'	TRIP
'h' 'c_p' 'volume' 'area'	Thermomechanical Coupling
'fc_' 'gx_' 'b5' 'b6' 'G1' 'G2' 'H1' 'H2' 'tw_a' 'tw_b';	Cyclic deformation

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Numerical Implementation

Subroutine Interface

'C_VARINTER' – give access to the list of names associated with the material's internal variables, LCVAR

```
LCVAR = LCHOOK  ET  LCR  ET   FININV  ET  BINT  ET  LCTAUP ET   LCG  ET  LGAM  ET  LCTAUTR  ET  LXI  ET  LXITOT
        ET LCTAUTW  ET  LCGW  ET  LXITW   ET   LXITWTOT   ET   LGAMTW   ET   LCTAUTRI  ET   LGAMTRIP   ET  LXIC
        ET   LTHETA  ET   LTMD  ET   LTLT   ET   LTH   ET   LGAMTOT   ET  LGAMTWOT ET  LGAMTROT  ET  LFC  ET  LGX;

LXI =   MOTS   'XI01'   'XI02'   'XI03'   'XI04'
               'XI05'   'XI06'   'XI07'   'XI08'
               'XI09'   'XI10'   'XI11'   'XI12'
               'XI13'   'XI14'   'XI15'   'XI16'
               'XI17'   'XI18'   'XI19'   'XI20'
               'XI21'   'XI22'   'XI23'   'XI24';
```

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Numerical Implementation

Time-integration Procedure

t: Prior Time

$\tau = t{+}\Delta t$: Current Time

Given:

(1) $\boldsymbol{F}(t)$,$\boldsymbol{F}(\tau)$, $\boldsymbol{F}_{inel}(t)$,

(2) $\boldsymbol{T}(t)$, $\boldsymbol{\sigma}(t)$,

(3) $\xi^{(i)}(t)$, $\xi_c(t)$,$\gamma_A^{(\alpha)}(t)$, $\gamma_{tw}^{(t)}(t)$, $\gamma_{trip}^{(\alpha)}(t)$,

$\tau_A^{(\alpha)}(t)$, $\tau_{tw}^{(t)}(t)$, $g_A^{(\alpha)}(t)$, $g_{tw}^{(t)}(t)$, $\boldsymbol{B}_{int}(t)$,

(4)$\theta(t)$

UMAT →

To Calculate:

(1) $\xi^{(i)}(\tau)$, $\xi_c(\tau)$, $\gamma_A^{(\alpha)}(\tau)$, $\gamma_{tw}^{(t)}(\tau)$, $\gamma_{trip}^{(\alpha)}(\tau)$,

$\tau_A^{(\alpha)}(\tau)$, $\tau_{tw}^{(t)}(\tau)$,. $g_A^{(\alpha)}(\tau)$,. $g_{tw}^{(t)}(\tau)$,. $\boldsymbol{B}_{int}(\tau)$,

(2) $\theta(\tau)$,

(3) $\boldsymbol{F}_{inel}(\tau)$,

(4) $\boldsymbol{T}(\tau)$, $\boldsymbol{\sigma}(\tau)$

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Numerical Implementation

Time-integration Procedure

Step1: Calculate $E_e(\tau)^{\text{trial}}$

$$F_e(\tau)^{trial} = F(\tau)F_{inel}(t)^{-1}$$
$$A(\tau)^{trial} = (F_e(\tau)^{trial})^T F_e(\tau)^{trial}$$
$$E_e(\tau)^{trial} = \frac{1}{2}(A(\tau)^{trial} - I)$$

Step2: Calculate elastic modulus

$$\mathbb{C}(t) = (1 - \xi(t))\mathbb{C}_A + \xi(t)\mathbb{C}_M$$

Step3: Calculate $T(\tau)^{\text{trial}}$, $\mathrm{M}(\tau)^{\text{trial}}$

$$T(\tau)^{trial} = \mathbb{C}(t) : E_e(\tau)^{trial}$$
$$M(\tau)^{trial} = A(\tau)^{trial} T(\tau)^{trial}$$

Step4: Calculate trial resolved shear stress

$$\tau_A{}^{(\alpha)}(\tau)^{trial} = M(\tau)^{trial} : S_p{}^{(\alpha)}$$
$$\tau_{tr}{}^{(i)}(\tau)^{trial} = (M(\tau)^{trial} + B_{int}(t)) : S_{tr}{}^{(i)}$$
$$\tau_{tw}{}^{(t)}(\tau)^{trial} = M(\tau)^{trial} : S_{tw}{}^{(t)}$$
$$\tau_{trip}{}^{(\alpha)}(\tau)^{trial} = (M(\tau)^{trial} + B_{int}(t)) : S_p{}^{(\alpha)}$$

Step5: Calculate trial driving force for each mechanism

$$f_{tr}^{(i)}(\tau)^{trial} = g_{tr}\tau_{tr}{}^{(i)}(\tau)^{trial} - \frac{1}{2}E_e : \Delta\mathbb{C}(t) : E_e - \mu(\theta(t) - \theta_0) - G\xi(t) - \frac{1}{2}\beta g_{tr}(1 - 2\xi(t))$$
$$f_A^{(\alpha)}(\tau)^{trial} = |\tau_A{}^{(\alpha)}(\tau)^{trial}| - g_A^{(\alpha)}(t)$$
$$f_{tw}^{(t)}(\tau)^{trial} = \tau_{tw}{}^{(t)}(\tau)^{trial} - g_{tw}^{(t)}(t)$$
$$f_{trip}^{(\alpha)}(\tau)^{trial} = \tau_{trip}{}^{(\alpha)}(\tau)^{trial}$$

Step6: Calculate $\Delta\gamma_A^{(\alpha)}(\tau)$, $\Delta\gamma_{tw}^{(t)}(\tau)$, $\Delta\xi^{(i)}(\tau)$ and $\Delta\gamma_{trip}^{(\alpha)}(\tau)$

Step7: Renew $\xi^{(i)}(\tau)$, $\xi(\tau)$ and $\xi_c(\tau)$

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Numerical Implementation

■ Time-integration Procedure

Step8: Calculate temperature change $\Delta\theta(\tau)$

Step9: Calculate and normalize $\boldsymbol{F}_{inel}(\tau)$

$$\boldsymbol{F}_{inel}(\tau) = [1 + (1-\xi(\tau))\sum_{\alpha=1}^{24}\Delta\gamma_A^{(\alpha)}(\tau)\boldsymbol{S}_p{}^{(\alpha)} + \sum_{i=1}^{24}\Delta\xi^{(i)}(\tau)g_{tr}\boldsymbol{S}_{tr}{}^{(i)} + \xi(\tau)\sum_{t=1}^{11}\Delta\gamma_{tw}^{(t)}(\tau)\boldsymbol{S}_{tw}{}^{(t)} + (1-\xi(\tau))\sum_{\alpha=1}^{24}\Delta\gamma_{trip}^{(\alpha)}(\tau)\boldsymbol{S}_p{}^{(\alpha)}]\boldsymbol{F}_{inel}(t)$$

$$\boldsymbol{J}_{inel} = det(\boldsymbol{F}_{inel}(\tau)),\ \ \boldsymbol{F}_{inel}(\tau) = \boldsymbol{J}_{inel}^{-\frac{1}{3}}\boldsymbol{F}_{inel}(\tau)$$

Step10: Update $\mathbb{C}(\tau)$

$$\mathbb{C}(\tau) = (1-\xi(\tau))\mathbb{C}_A + \xi(t)\mathbb{C}_M$$

Step11: Compute $\boldsymbol{F}_e(\tau)$, $\boldsymbol{T}(\tau)$and$\boldsymbol{\sigma}(\tau)$

$$\boldsymbol{F}_e(\tau) = \boldsymbol{F}(\tau)\boldsymbol{F}_{inel}(\tau)^{-1}$$

$$\boldsymbol{T}(\tau) = \mathbb{C}(\tau) : \boldsymbol{E}_e(\tau)$$

$$\boldsymbol{\sigma} = \frac{1}{det(\boldsymbol{F}_e(\tau))}\boldsymbol{F}_e(\tau)\boldsymbol{T}(\tau)(\boldsymbol{F}_e(\tau))^T$$

Step12: Renew a group of internal variables

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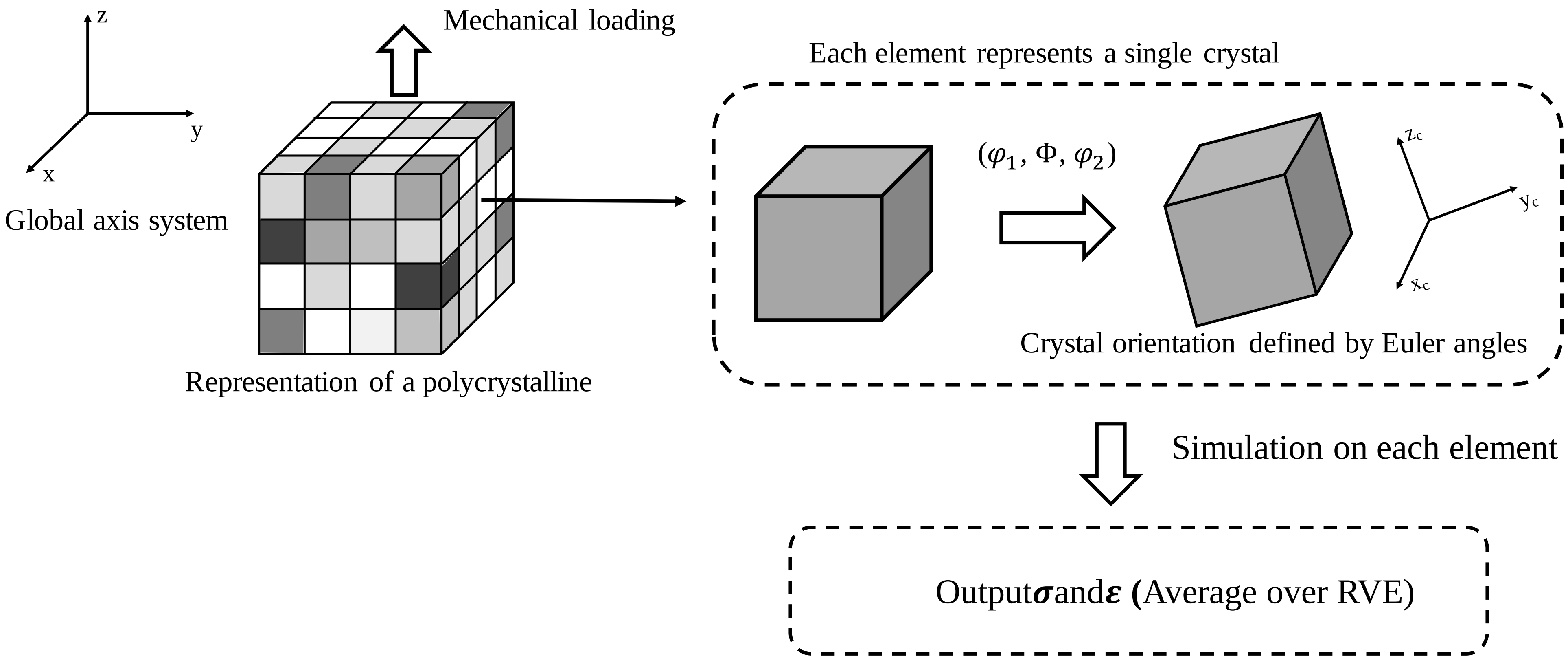
Numerical Implementation

Generalize the Model for Polycrystalline



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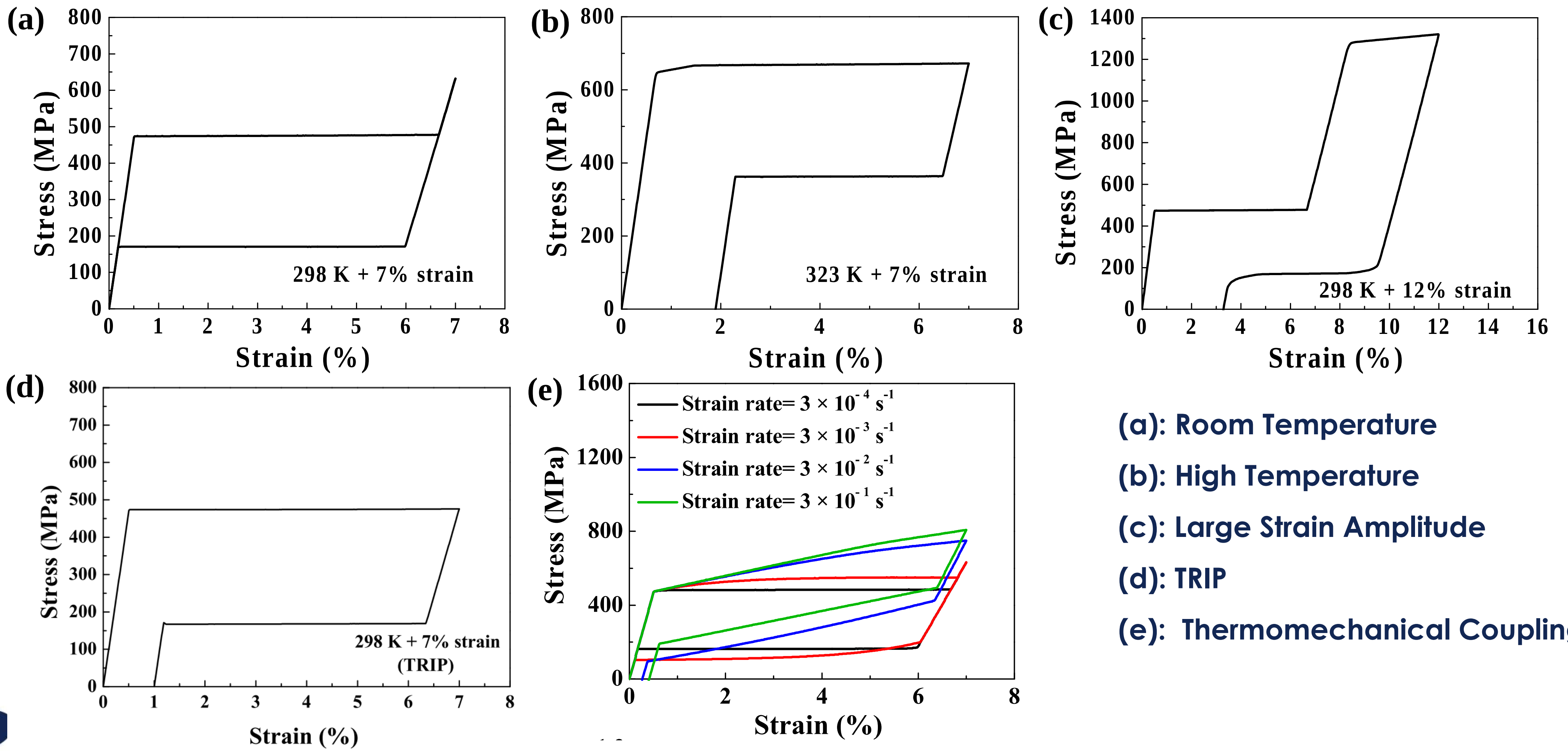
Selected Results

- Activation of inelastic mechanisms



(a): Room Temperature

(b): High Temperature

(c): Large Strain Amplitude

(d): TRIP

(e): Thermomechanical Coupling

Ju X, Moumni Z, Zhang Y, et al. International Journal of Plasticity, 2022.

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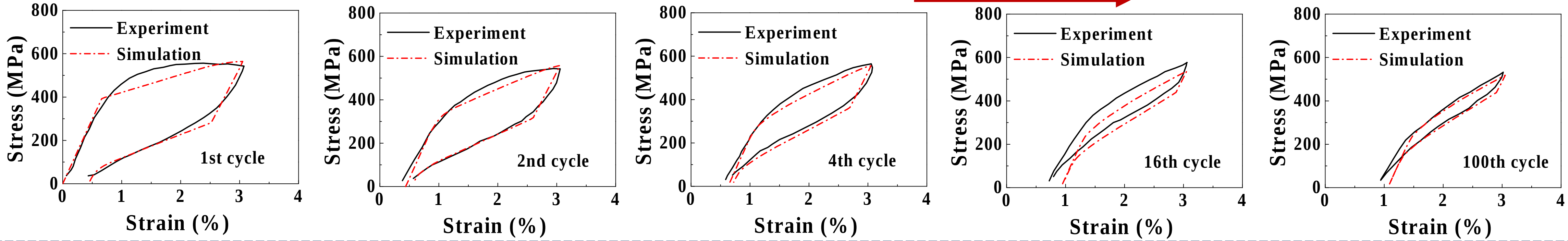
Selected Results

■ Cyclic Responses of Single Crystal of Different Orientations

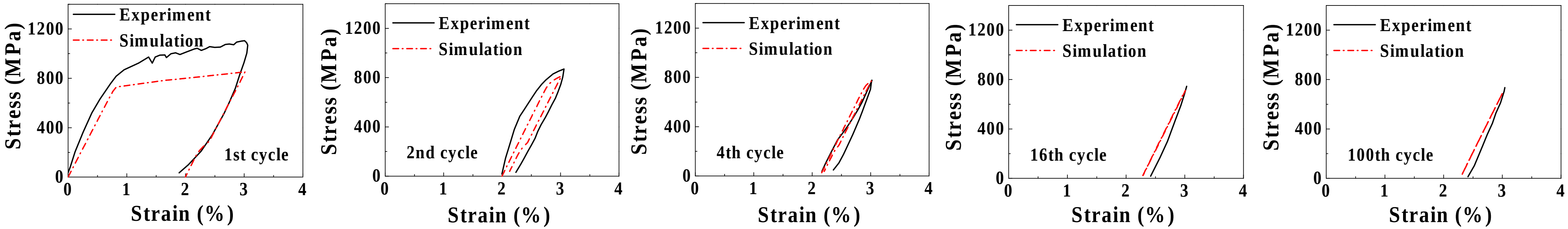
Loading cycles →

Gall K, Maier H J. Acta Materialia, 2002

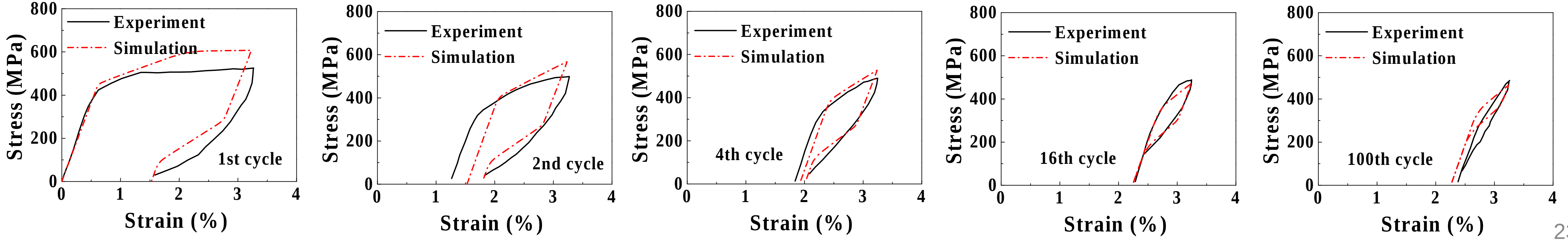
[210]



[111]



[321]



Ju X, Moumni Z, Zhang Y, et al. International Journal of Plasticity, 2022.

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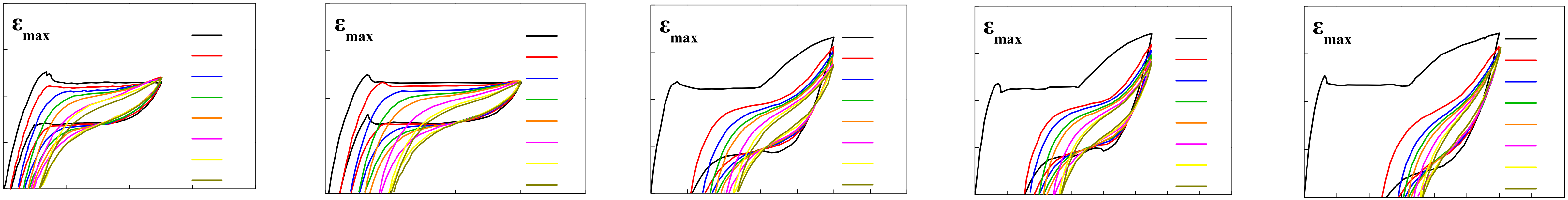
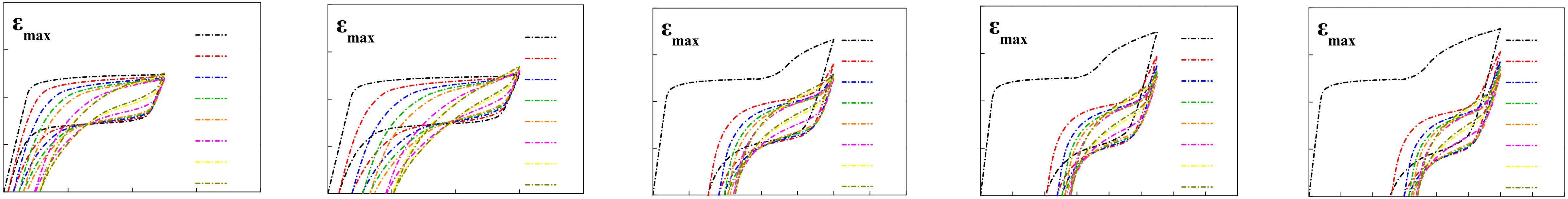
Selected Results

- **Cyclic Responses of Polycrystalline at Different Strain Amplitudes**

Experiment (Wang et al., 2008)



Our Simulation (γ- fiber {111})



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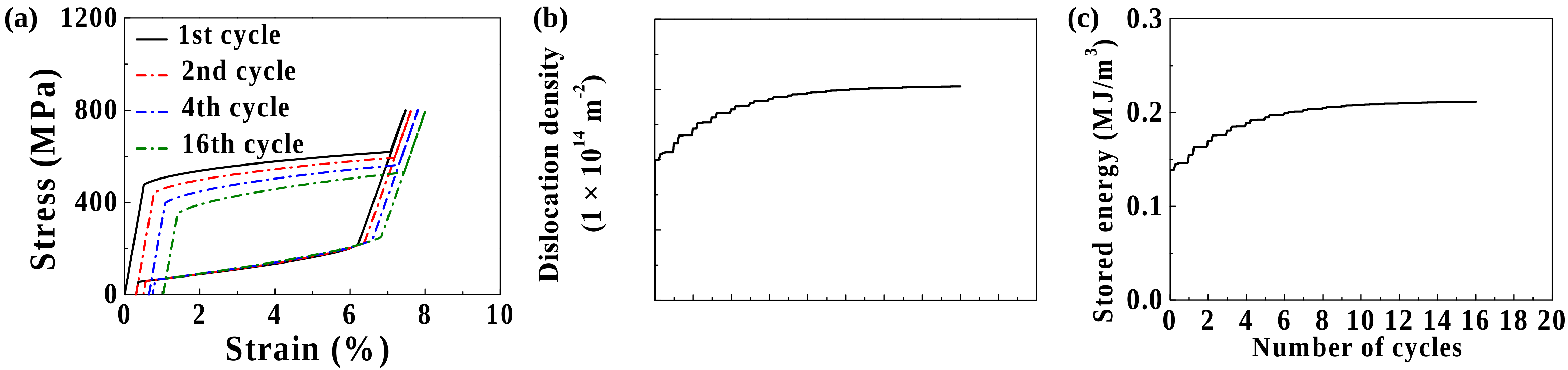
Selected Results

■ Evolution of Microstructural-related Variables



$$\rho_{tot} = (1-\xi)\rho_A + \xi \cdot \xi_{tw} \cdot \rho_M,$$

$$E_{st} \approx \rho_{tot} E_{dis} \approx \frac{1}{2}\rho_{tot} G_{shear} b^2$$

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Ju X, Moumni Z, Zhang Y, et al. International Journal of Plasticity, 2022.

Conclusions

- Developed a Multiscale and Thermomechanical Model for SMAs
- Implemented the model into CAST3M and Well Reproduced Cyclic Response of SMAs
- Introduced Variables Associated with Microstructural Changes for Fatigue Analysis

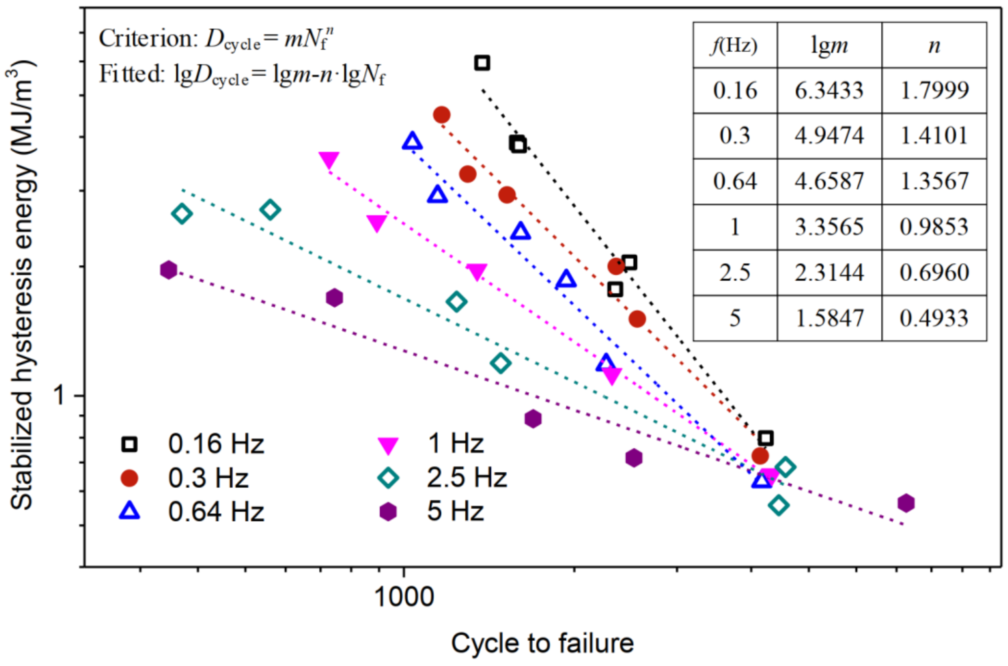
Thank you for your attention!

PhD student (Reporter): **Xiaofei JU** (xiaofei.ju@ensta-paris.fr)

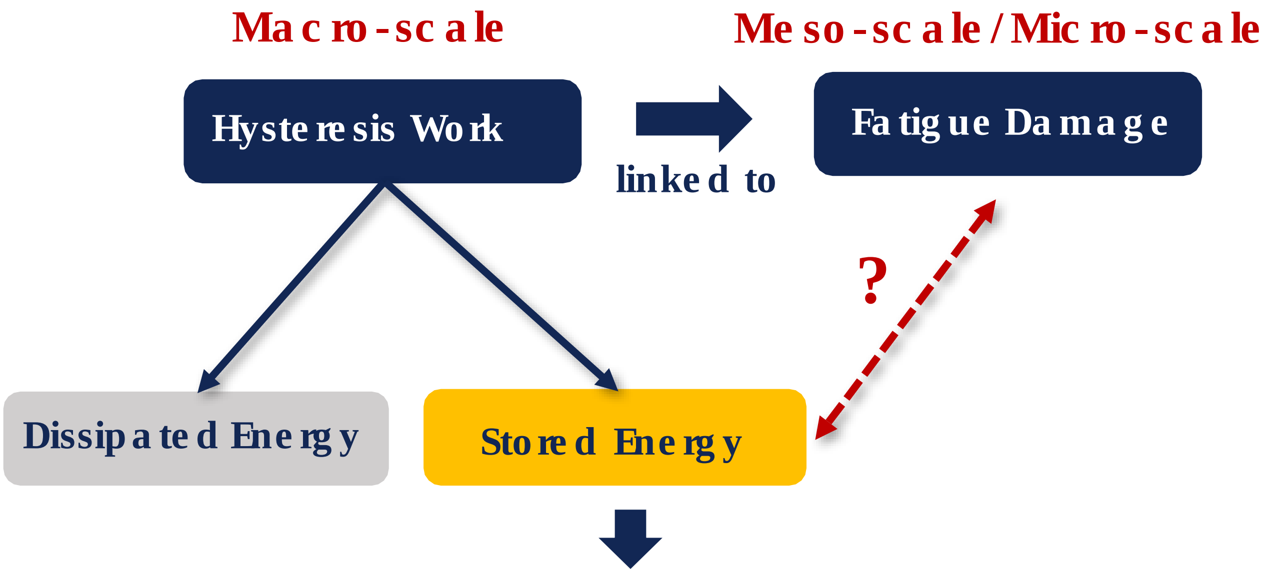
Supervisor: **Ziad MOUMNI** (ziad.moumni@ensta-paris.fr)

Motivations

■ Development of a Reliable Fatigue Criterion



f(Hz)	lgm	n
0.16	6.3433	1.7999
0.3	4.9474	1.4101
0.64	4.6587	1.3567
1	3.3565	0.9853
2.5	2.3144	0.6960
5	1.5847	0.4933



Intrinsic Indicator for Fatigue Behavior ?

For NiTi SMAs:

$$D_{cycle} = m_1 f^{m_2} N_f^{(n_1 \cdot \lg f + n_2)}$$

Micromechanical-based Models are the key for Investigating the fatigue behavior & further establishing a good fatigue criterion

Zhang Y. Low cycle fatigue of shape memory alloys [phd thesis]. 2018

Equations

- **Definition of Effective Anisotropic Elastic Moduli**

$$\mathbb{C} = (1 - \xi)\mathbb{C}_A + \xi\mathbb{C}_M$$

$$\boldsymbol{T} = \mathbb{C} : \boldsymbol{E}_e$$

$$\boldsymbol{\sigma} = \frac{1}{det(\boldsymbol{F}_e)} \boldsymbol{F}_e \boldsymbol{T} \boldsymbol{F}_e^T$$

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Equations

- **Thermomechanical Coupling**

The first law of thermodynamics

$$\dot{U} = \boldsymbol{P}:\dot{\boldsymbol{F}} - \nabla \cdot \boldsymbol{q} \quad \xrightarrow{\psi = U - \theta q} \quad \theta\dot{\eta} = \boldsymbol{P}:\dot{\boldsymbol{F}} - \dot{\psi} - \dot{\theta}\eta - \nabla \cdot \boldsymbol{q}$$

$$\boldsymbol{P} : \dot{\boldsymbol{F}} = \boldsymbol{T} : \dot{\boldsymbol{E}}_e + \boldsymbol{F}_e^T \boldsymbol{F}_e \boldsymbol{T} : \boldsymbol{L}_{inel}$$

$$\theta\dot{\eta} = \sum_{i=1}^{24} f_{tr}^{(i)} \dot{\xi}^{(i)} + (1-\xi) \sum_{\alpha=1}^{24} f_A^{(\alpha)} \dot{\gamma}_A^{(\alpha)} + \xi \sum_{t=1}^{11} f_{tw}^{(t)} \dot{\gamma}_{tw}^{(t)} + (1-\xi) \sum_{\alpha=1}^{24} f_{trip}^{(\alpha)} \dot{\gamma}_{trip}^{(\alpha)} - \nabla \cdot \boldsymbol{q}$$

$$\eta = -\frac{\partial\psi}{\partial\theta} = C \ln\frac{\theta}{\theta_0} - \mu \sum_{i=1}^{24} \xi^{(i)}$$

$$C\dot{\theta} + \nabla \cdot \boldsymbol{q} = \underbrace{\sum_{i=1}^{24} f_{tr}^{(i)} \dot{\xi}^{(i)} + (1-\boldsymbol{\xi}) \sum_{\alpha=1}^{24} f_A^{(\alpha)} \dot{\gamma}_A^{(\alpha)} + \xi \sum_{t=1}^{11} f_{tw}^{(t)} \dot{\gamma}_{tw}^{(t)} + (1-\xi) \sum_{\alpha=1}^{24} f_{trip}^{(\alpha)} \dot{\gamma}_{trip}^{(\alpha)}}_{Mechanical\ dissipation} + \underbrace{\theta\mu \sum_{i=1}^{24} \dot{\xi}^{(i)}}_{Latent\ heat}$$

Simulation Part – Basic Model

Helmholtz free energy density

$$\psi\left(\boldsymbol{E}_e, \xi^{(i)}, \theta\right) = \psi_e + \psi_\theta + \psi_{int} + \psi_p + \psi_{trans} + \psi_{cst}$$

where,

$$\psi_e = \frac{1}{2}\boldsymbol{E}_e : \mathbb{C} : \boldsymbol{E}_e$$

$$\psi_\theta = C\left[(\theta - \theta_0) - \theta \ln \frac{\theta}{\theta_0}\right] + \mu(\theta - \theta_0)\xi$$

$$\dot{\psi}_{int} = -\boldsymbol{B}_{int} : \left(\boldsymbol{L}_{tr} + \boldsymbol{L}_{trip}\right)$$

$$\dot{\psi}_p = (1-\xi)\sum_{\alpha=1}^{24} g_A^{(\alpha)}\left|\dot{\gamma}_A^{(\alpha)}\right| + \xi \sum_{t=1}^{11} g_{tw}^{(t)}\left(\dot{\gamma}_{tw}^{(t)}\right)$$

$$\psi_{trans} = \frac{1}{2}G\xi^2 + \frac{1}{2}\beta g_{tr}\xi(1-\xi)$$

$$\psi_{cst} = -w_0(1-\xi) - \sum_{i=1}^{N_T} w_i \xi^{(i)}$$

Thermodynamic Driving Forces

$$\boldsymbol{P} : \dot{\boldsymbol{F}} - \dot{\psi} - \eta\dot{\theta} - \frac{\boldsymbol{q}\nabla\theta}{\theta} \geq 0$$

Clausius-Duhem Inequality

$$\underbrace{\left(\boldsymbol{T} - \frac{\partial\psi}{\partial \boldsymbol{E}_e}\right)}_{=0} : \dot{\boldsymbol{E}}_e - \underbrace{\left(\eta + \frac{\partial\psi}{\partial\theta}\right)}_{=0}\dot{\theta} + \underbrace{\sum_{i=1}^{24}\left[g_{tr}(\boldsymbol{M} + \boldsymbol{B}_{int}) : \boldsymbol{S}_{tr}^{(i)} - \frac{\partial\psi}{\partial\xi^{(i)}}\right]\dot{\xi}^{(i)}}_{\geq 0}$$

$$+ \underbrace{(1-\xi)\sum_{\alpha=1}^{24}\left[\left(\boldsymbol{M} : \boldsymbol{S}_p{}^{(\alpha)}\right)\dot{\gamma}_A^{(\alpha)} - g_A^{(\alpha)}\left|\dot{\gamma}_A^{(\alpha)}\right|\right]}_{\geq 0} + \underbrace{\xi\sum_{t=1}^{11}\left(\boldsymbol{M} : \boldsymbol{S}_{tw}{}^{(t)} - g_{tw}^{(t)}\right)\dot{\gamma}_{tw}^{(t)}}_{\geq 0}$$

$$+ \underbrace{(1-\xi)\sum_{\alpha=1}^{24}\left[(\boldsymbol{M} + \boldsymbol{B}_{int}) : \boldsymbol{S}_p{}^{(\alpha)}\right]\dot{\gamma}_{trip}^{(\alpha)}}_{\geq 0} - \underbrace{\frac{\boldsymbol{q}\nabla\theta}{\theta}}_{\geq 0} \geq 0$$

Thermodynamic Driving Force For Phase Transformation

$$f_{tr}^{(i)} = g_{tr}(\boldsymbol{M} + B_{int}) : \boldsymbol{S}_{tr}{}^{(i)} - \frac{1}{2}\boldsymbol{E}_e : \Delta\mathbb{C} : \boldsymbol{E}_e - \mu(\theta - \theta_0)$$

$$-G\xi - \frac{1}{2}\beta g_{tr}(1 - 2\xi) + w_0 - w_i$$

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Implementation

- **Detailed procedure for step 6**
  - Plasticity in austenite

(1) The slip increment is approximated as:

$$\Delta\gamma_A^{(\alpha)}(\tau) \approx [(1-\theta_1)\dot{\gamma}_A^{(\alpha)}(t) + \theta_1\dot{\gamma}_A^{(\alpha)}(\tau)]\Delta t$$

(θ_1 is a parameter between [0, 1]. In the present work, θ_1 is taken as 0.5.)

(2) Employing a Taylor expansion:

$$\dot{\gamma}_A^{(\alpha)}(\tau) = \dot{\gamma}_A^{(\alpha)}(t) + \left.\frac{\partial\dot{\gamma}_A^{(\alpha)}}{\partial\tau_A^{(\alpha)}}\right|_t \Delta\tau_A^{(\alpha)}(\tau) + \left.\frac{\partial\dot{\gamma}_A^{(\alpha)}}{\partial g_A^{(\alpha)}}\right|_t \Delta g_A^{(\alpha)}(\tau)$$

(3) The slip increment is rewritten as:

$$\Delta\gamma_A^{(\alpha)}(\tau) = \Delta t\left(\dot{\gamma}_A^{(\alpha)}(t) + \theta_1 \left.\frac{\partial\dot{\gamma}_A^{(\alpha)}}{\partial\tau_A^{(\alpha)}}\right|_t \Delta\tau_A^{(\alpha)}(\tau) + \theta_1 \left.\frac{\partial\dot{\gamma}_A^{(\alpha)}}{\partial g_A^{(\alpha)}}\right|_t \Delta g_A^{(\alpha)}(\tau)\right)$$

Where, $\Delta\tau_A^{(\alpha)}(\tau) = \tau_A^{(\alpha)}(\tau)^{trial} - \tau_A^{(\alpha)}(t)$, $\Delta g_A^{(\alpha)}(\tau) = \sum_{\beta=1}^{24} h_A^{\alpha\beta}\left|\Delta\gamma_A^{(\beta)}(\tau)\right|$

Explicit method

(4) $f\left(\Delta\gamma_A^{(\alpha)}(\tau)\right) \doteq \Delta\gamma_A^{(\alpha)}(\tau) - [(1-\theta_1)\dot{\gamma}_A^{(\alpha)}(t) + \theta_1\dot{\gamma}_A^{(\alpha)}(\tau)]\Delta t$

(5) solve $f\left(\Delta\gamma_A^{(\alpha)}(\tau)\right) \doteq 0$ by Newton-Raphson method

Implicit method

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Implementation

Detailed procedure for step 6

- Phase transformation

(1) Determine the set of potentially active systems $\mathcal{PA}$

a. For forward transformation, the system belongs to $\mathcal{PA}$ if it satisfies:

$$f_{tr}^{(i)}(\tau)^{trial} - f_c^{(i)} > 0\,, \qquad \xi^{(i)}(t) \in [0,1) \qquad \text{and} \qquad \xi(t) \in [0,1)$$

b. For reverse transformation, the system belongs to $\mathcal{PA}$ if it satisfies:

$$f_{tr}^{(i)}(\tau)^{trial} + f_c^{(i)} < 0\,, \qquad \xi^{(i)}(t) \in (0,1] \qquad \text{and} \qquad \xi(t) \in (0,1]$$

(2) Solve a equation set deriving from the consistency conditions: $\sum_{j\in\mathcal{PA}} A^{ij} x^j = b^i \,, i \in \mathcal{PA}$

a. For the forward phase transformation, it has:

$$A^{ij} = [g_{tr}{}^2 \boldsymbol{C}_{trans}^{(j)}(\tau)^{trial} - \textstyle\sum_{k=1}^{24}(\frac{B_{sat}}{b} e^{-\frac{\xi_c(t)}{b}} \boldsymbol{S}_{tr}^{(k)})] : \boldsymbol{S}_{tr}^{(i)} + G - \beta g_{tr}$$

$$b^i = f_{tr}^{(i)}(\tau)^{trial} - f_c^{(i)}$$

$$x^i = \Delta\xi^{(i)}(\tau) > 0$$

b. For the reverse phase transformation, it has:

$$A^{ij} = [g_{tr}{}^2 \boldsymbol{C}_{trans}^{(j)}(\tau)^{trial} + \textstyle\sum_{k=1}^{24}(\frac{B_{sat}}{b} e^{-\frac{\xi_c(t)}{b}} \boldsymbol{S}_{tr}^{(k)})] : \boldsymbol{S}_{tr}^{(i)} + G - \beta g_{tr}$$

$$b^i = f_{tr}^{(i)}(\tau)^{trial} + f_c^{(i)}$$

$$x^i = \Delta\xi^{(i)}(\tau) < 0$$

(3) If the solution $\Delta\xi^{(i)}(\tau)$ is negative during forward transformation, this system is inactive and removed from $\mathcal{PA}$. A^{ij} will be recalculated.
Similar conduction for reverse transformation (when $\Delta\xi^{(i)}(\tau)$ positive).

(4) Such iterative procedure is continued until all $\Delta\xi^{(i)}(\tau)$ satisfy the requirement.

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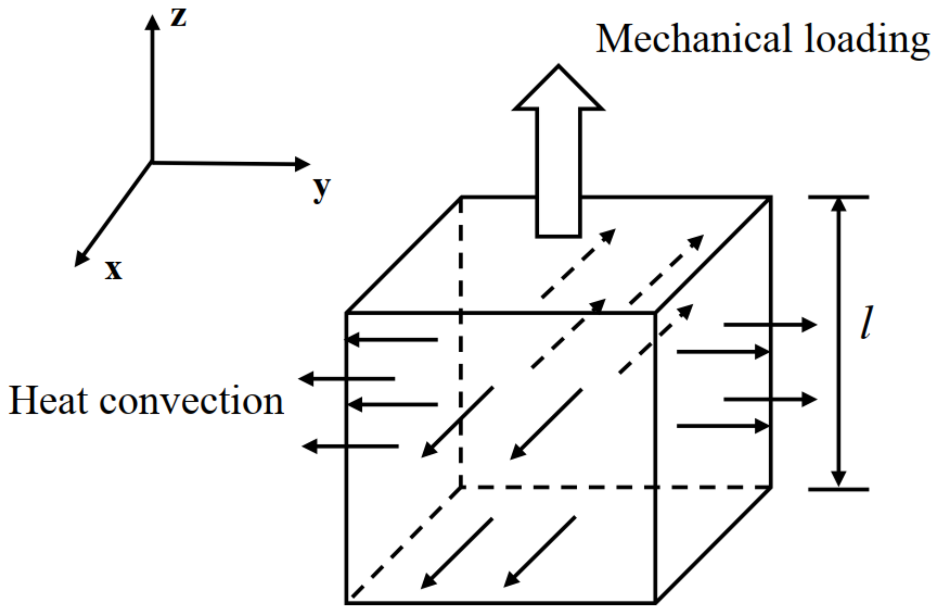
Implementation

Boundary Conditions



$u_z(z=0)=0$
$u_x(x=0)=0$
$u_y(y=0)=0$
$u_z(z=l)=u_z(t)$

```
csu = enve vol1;
x1 = coor vol1 1;
haut = csu elem 'APPU' 'STRI' (x1 poin 'EGAL' l1) coul bleu;


cl_haut = bloq 'UX' haut;
depx = DEPI cl_haut (50.*l3);

ltps = prog 0.  234.;
lamp = prog 0. 0.001;
ev1 = evol 'MANU'  ltps  lamp;

cha0 = CHAR 'DIMP' depx ev1;


rigx = bloq sur1 'UX';


x2 = coor vol1 2;
symy = csu elem 'APPU' 'STRI' (x2 poin 'EGAL' 0.) coul roug;
d4 = d4 coul roug;
rigy = BLOQ d4 'UY';

x3 = coor vol1 3;
symz = csu elem 'APPU' 'STRI' (x3 poin 'EGAL' 0.) coul vert;
d1 = d1 coul vert;
rigz = BLOQ d1 'UZ';
```

Implementation

Pasapas

```
cl_haut = bloq 'UX' haut;
depx = DEPI cl_haut (50.*l3);

ltps = prog 0.  234.;
lamp = prog 0. 0.001;
ev1 = evol 'MANU'  ltps  lamp;

cha0 = CHAR 'DIMP' depx ev1;
```

Displacement Control Loading

```
TABU = TABLE ;
TABU.'MODELE' = mo_util ;
TABU.'CARACTERISTIQUES' = ma_util1 et ma_util2 ;
TABU.GRANDE_DEPLACEMENTS= vrai;
TABU.'BLOCAGES_MECANIQUES' = rigx et rigy et rigz et cl_haut;
TABU.'CHARGEMENT' = cha0 ;
TABU.'TEMPS_CALCULES' = PROG 0. pas 0.02 234.;
TABU.'TEMPS_SAUVES' = PROG 0. pas 2. 234.;
TMASAU=table;
tabu . 'MES_SAUVEGARDES'=TMASAU;
TMASAU .'DEFTO'=VRAI;
TMASAU .'DEFIN'=VRAI;
TEMPS 'ZERO' ;
PASAPAS TABU ;
```

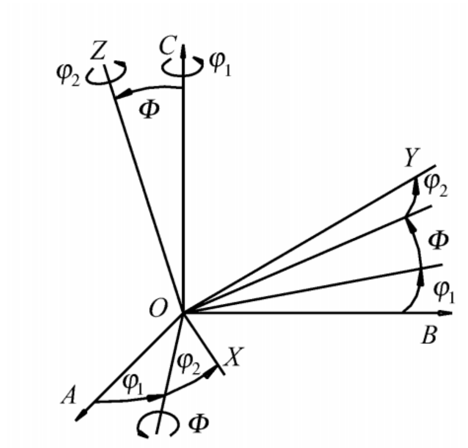
```
tt=tabu. TEMPS_SAUVES;
nn= dime tt ;
nn=nn-1;

*N = dime (tabu.DEPLACEMENTS);
ff= prog 0.;
repe BOUC1 ne;
repe BOUC2 8;

SI ((&BOUC1 < 2) ET (&BOUC2 < 2));
ff= extr (tabu. contraintes. nn) smxx 1 &BOUC1 &BOUC2;

SINON;

ff= ff + (extr(tabu. contraintes. nn) smxx 1 &BOUC1 &BOUC2);

FINSI;

fin BOUC2;
fin BOUC1;
ff=ff/nip;

ltps2 = prog 234. 468.;
lamp2 = prog 1.  0.08;
ev2 = evol 'MANU'  ltps2  lamp2;
```

Force-control Unloading

```
flot1=flot (-1.*ff);
f1=pres mass mo_util flot1 haut;
cha2= CHAR 'MECA' f1 ev2;

TABU.'BLOCAGES_MECANIQUES' = rigx et rigy et rigz;
TABU.'CHARGEMENT' = cha2 ;
TABU.'TEMPS_CALCULES' = PROG 234. pas 0.02 468.;
TABU.'TEMPS_SAUVES' = PROG 234. pas 2. 468.;
*TABU.'CONTRAINTES' .0= si1;
TMASAU=table;
tabu . 'MES_SAUVEGARDES'=TMASAU;
TMASAU .'DEFTO'=VRAI;
TMASAU .'DEFIN'=VRAI;
TEMPS 'ZERO' ;
PASAPAS TABU ;

*TABTPS = TEMP 'NOEC';
*CPUext = TABTPS.'TEMPS_CPU'.'INITIAL';

opti sauv '1cycle.sauv';
SAUV tabu;
```

Euler Angles

■ Use Euler angles to represent the transformation matrix



- **ABC- Global coordinate system**
- **XYZ- Local coordinate system**

- **Rotate sequence: Z-X-Zwiththeangleof(φ_1,ϕ, φ_2)**

$$g=\begin{bmatrix}\cos\varphi_2 & \sin\varphi_2 & 0\\ -\sin\varphi_2 & \cos\varphi_2 & 0\\ 0 & 0 & 1\end{bmatrix}\begin{bmatrix}1 & 0 & 0\\ 0 & \cos\Phi & \sin\Phi\\ 0 & -\sin\Phi & \cos\Phi\end{bmatrix}\begin{bmatrix}\cos\varphi_1 & \sin\varphi_1 & 0\\ -\sin\varphi_1 & \cos\varphi_1 & 0\\ 0 & 0 & 1\end{bmatrix} \quad (1\text{-}5)$$

- **Transport of the transformation matrix**

$$g=\begin{bmatrix}\cos\varphi_1\cos\varphi_2-\sin\varphi_1\sin\varphi_2\cos\Phi & \sin\varphi_1\cos\varphi_2+\cos\varphi_1\sin\varphi_2\cos\Phi & \sin\varphi_2\sin\Phi\\ -\cos\varphi_1\sin\varphi_2-\sin\varphi_1\cos\varphi_2\cos\Phi & -\sin\varphi_1\sin\varphi_2+\cos\varphi_1\cos\varphi_2\cos\Phi & \cos\varphi_2\sin\Phi\\ \sin\varphi_1\sin\Phi & -\cos\varphi_1\sin\Phi & \cos\Phi\end{bmatrix}$$

$$=\begin{bmatrix}u & r & h\\ v & s & k\\ w & t & l\end{bmatrix} \quad (1\text{-}6)$$

- **Rangeoftheangles**

$\varphi_1 \in [0, 2\pi]$, $\phi \in [0, \pi]$, $\varphi_2 \in [0, 2\pi]$

Random Orientation

- **Range of the angles**

$\varphi_1 \in [0, 2\pi], \quad \phi \in [0, \pi], \quad \varphi_2 \in [0, 2\pi]$

- **Code in dgibi file**

```
fai1 thta fai2 = 0. 0. 0.;
fai1=BRUI 'BLAN' 'UNIF' 180. 180. (nbel vol1);
thta=BRUI 'BLAN' 'UNIF' 90. 90. (nbel vol1);
fai2=BRUI 'BLAN' 'UNIF' 180. 180. (nbel vol1);
```

Generate a random value list in the defined range for the Euler angles

```
opti 'SORT' 'fai1_n3';
SORT 'EXCE' fai1;
opti 'SORT' 'thta_n3';
SORT 'EXCE' thta;
opti 'SORT' 'fai2_n3';
SORT 'EXCE' fai2;
```

Output the random value list for the Euler angles

```
fai1= manu 'CHML'  mo_util 'REPA' 'TYPE' 'RIGIDITE'  'fai1' fai1;
thta= manu 'CHML'  mo_util 'REPA' 'TYPE' 'RIGIDITE'  'thta' thta;
fai2= manu 'CHML'  mo_util 'REPA' 'TYPE' 'RIGIDITE'  'fai2' fai2;
```

Spread the values of Euler angles on each element

Random Orientation

- **Generate pole figure from Euler angles (to check the orientations generated by simulations)**

Use MTEX Toolbox

- **Code in Matlab**

```
**********************************************
*text redine wobble angle of 5 degree of {111}<110>
cs=crystalSymmetry('m3m');
ss=specimenSymmetry('1');
fname=[mtexDataPath '/ODF/euler_n5.txt' ];
ori = loadOrientation_generic(fname,'CS',cs,'SS',ss, 'ColumnNames', {'Euler1' 'Euler2' 'Euler3'},'Columns',[1,2,3],'Degrees','Bunge');
setMTEXpref('xAxisDirection','north');
setMTEXpref('zAxisDirection','outofPlane');
plotPDF(ori,Miller({1,0,0},{1,1,1},{1,1,0},cs),'MarkerSize', 3,'points','all');
```

1. **Define the symmetry of crystal and specimen**
2. **Input the Euler angles in the form of txt file.**
3. **Read the txt file as orientations**
4. **Set the direction for the pole figure**
5. **Plot the pole figure in the crystallographic orientations**

Texture

- Range of the angles (<111>{1-10} texture)

=> [111], [1-10], [11-2]

=> $\varphi_1=0, \phi=55°, \varphi_2=45°$

consider wobble angle for polycrystal

$\varphi_1 \in [0, 360°], \ \phi = 55° \pm 5°, \ \varphi_2 = 45°$

- Code in dgibi file

```
fai1 thta fai2 = 0. 0. 45.;
fai1=BRUI 'BLAN' 'UNIF' 180. 180. (nbel vol1);
thta=BRUI 'BLAN' 'UNIF' 55. 5. (nbel vol1);
*fai2=BRUI 'BLAN' 'UNIF' 180. 180. (nbel vol1);
```

Generate a random value list in the defined range for the Euler angles

```
opti 'SORT' 'fai1_n5';
SORT 'EXCE' fai1;
opti 'SORT' 'thta_n5';
SORT 'EXCE' thta;
```

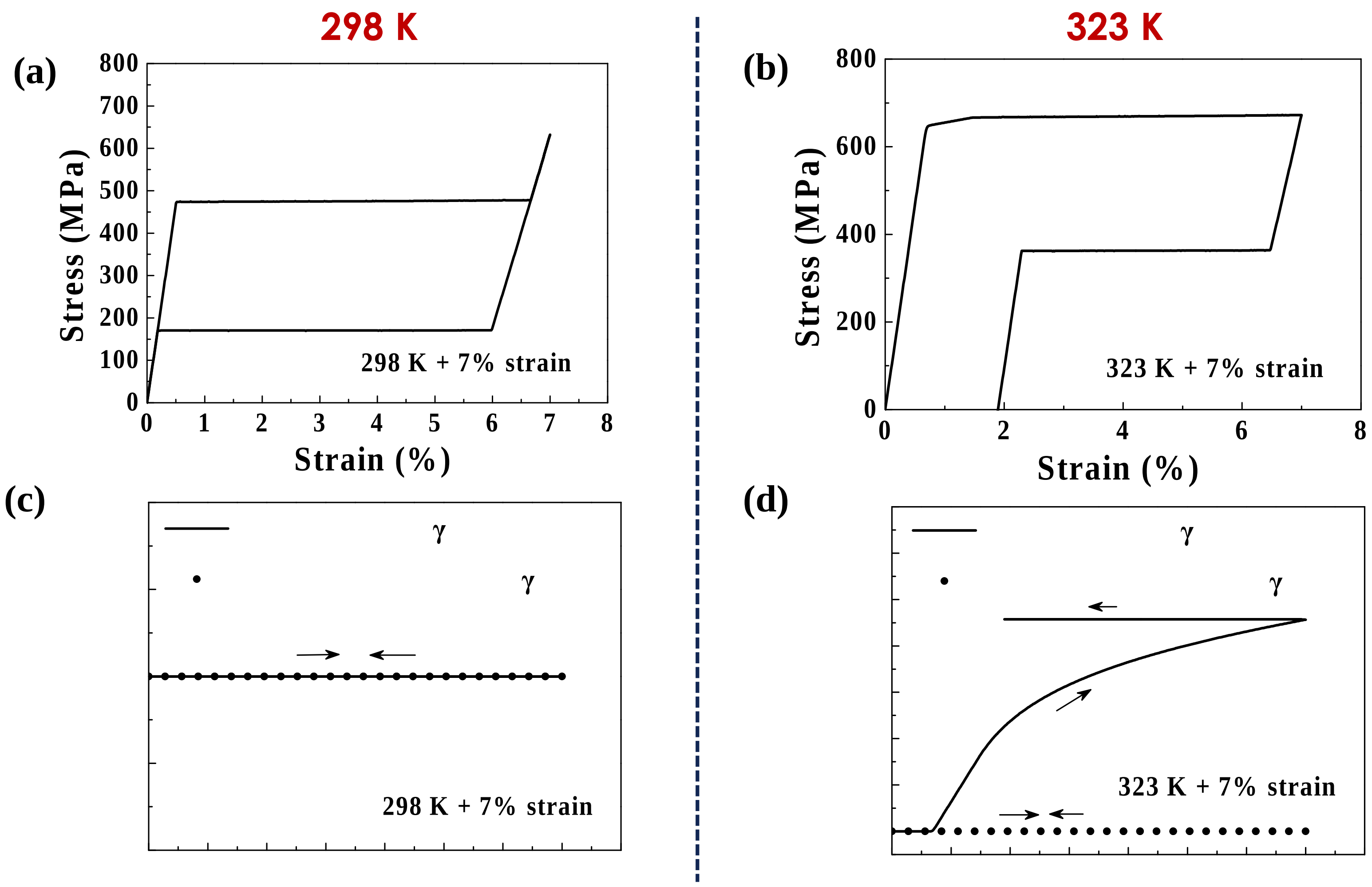
Output the random value list for the Euler angles

```
fai1= manu 'CHML'  mo_util 'REPA' 'TYPE' 'RIGIDITE'  'fai1' fai1;
thta= manu 'CHML'  mo_util 'REPA' 'TYPE' 'RIGIDITE'  'thta' thta;
*fai2= manu 'CHML'  mo_util 'REPA' 'TYPE' 'RIGIDITE'  'fai2' fai2;
```

Spread the values of Euler angles on each element

Results

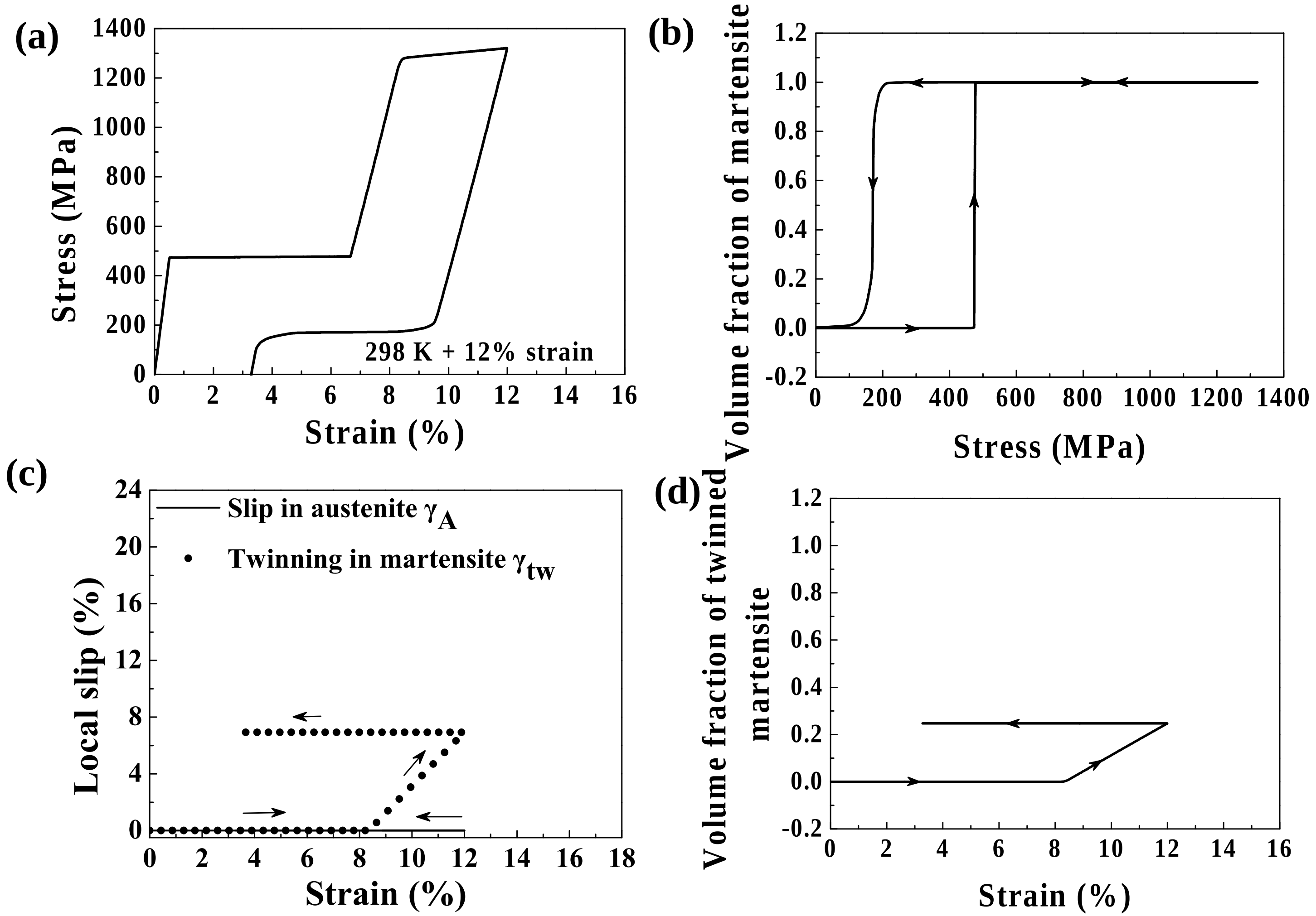
■ **Deformation slip in austenite at high temperature**



Ju X, Moumni Z, Zhang Y, et al. International Journal of Plasticity, 2022.

Results

- **Deformation twinning in martensite at large strain**



Ju X, Moumni Z, Zhang Y, et al. International Journal of Plasticity, 2022.

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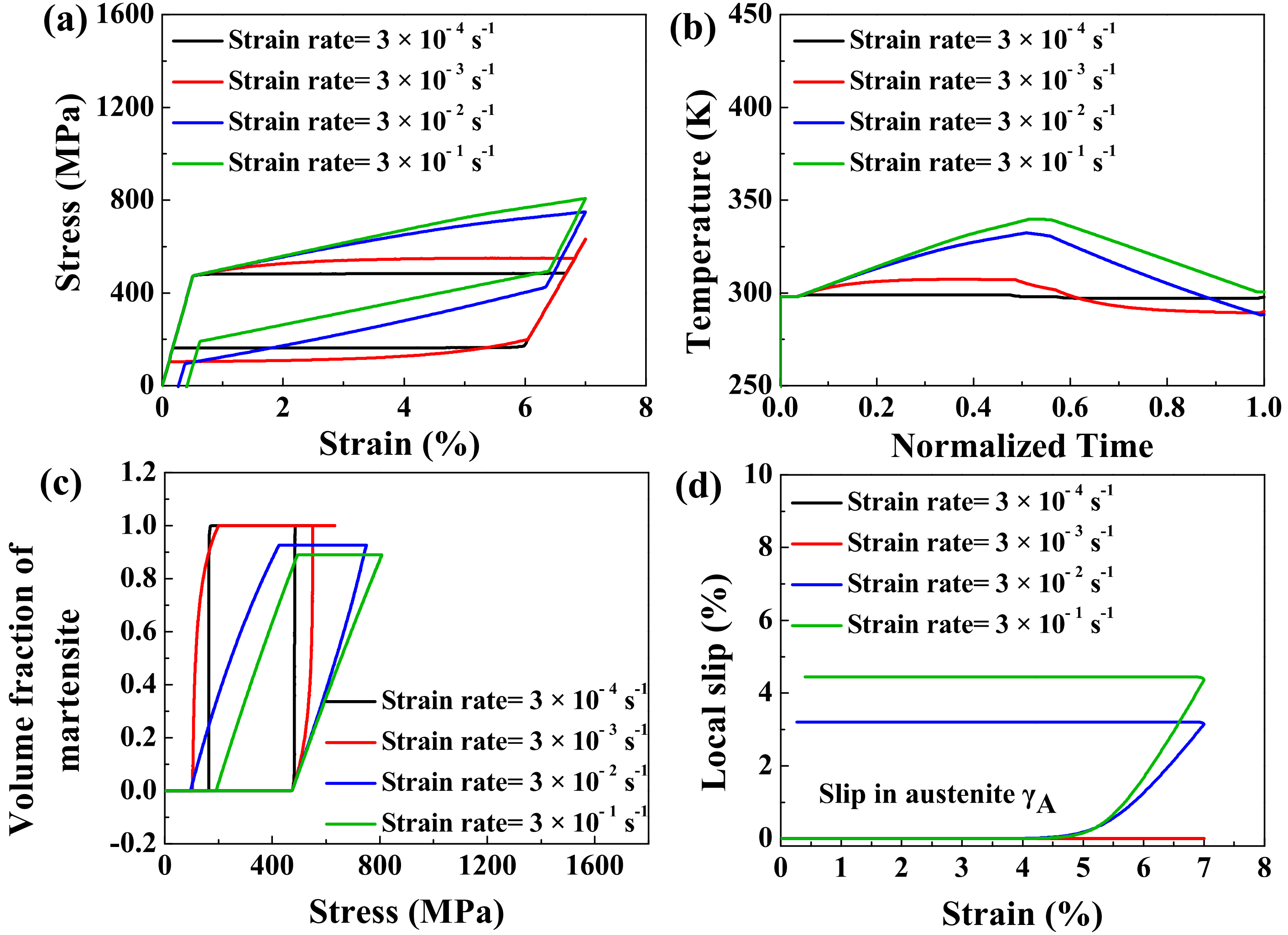
Results

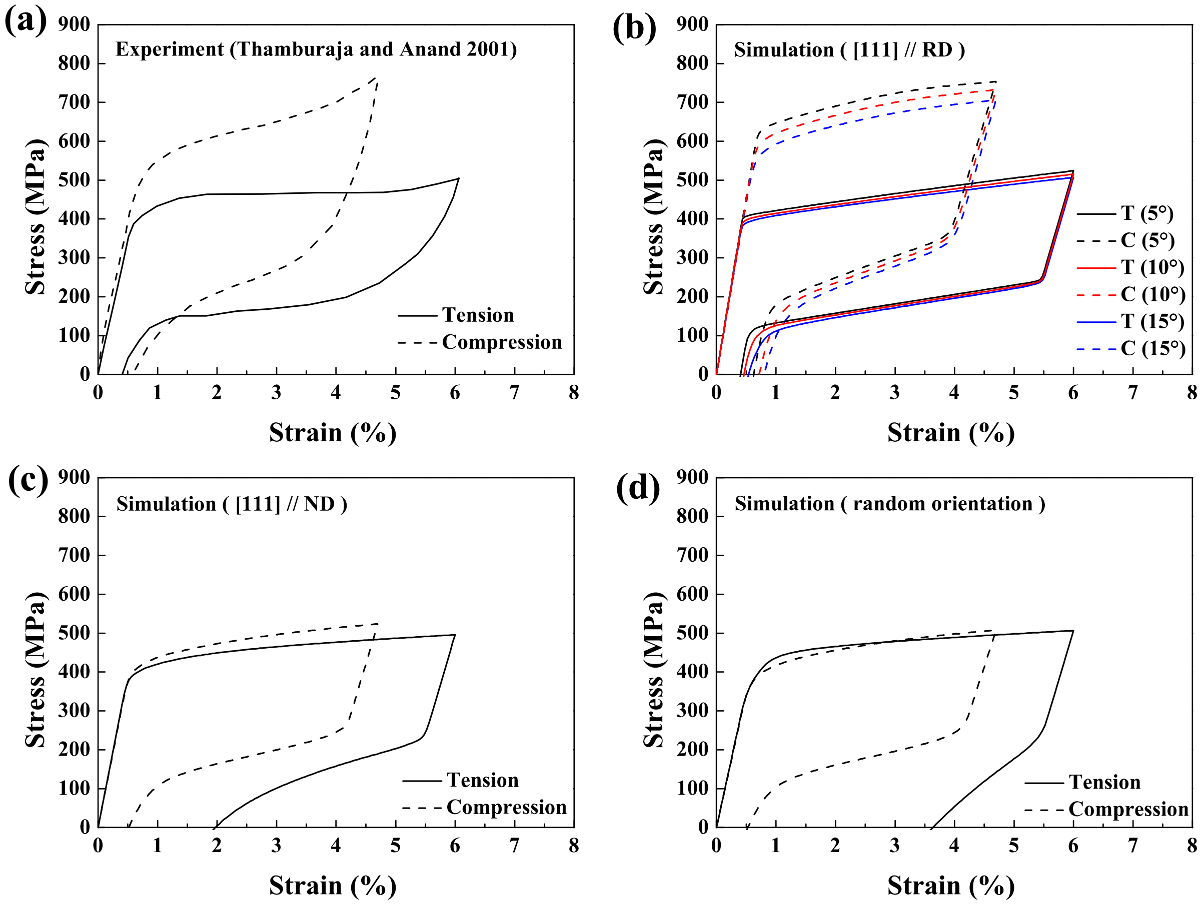
- **Thermomechanical coupling**



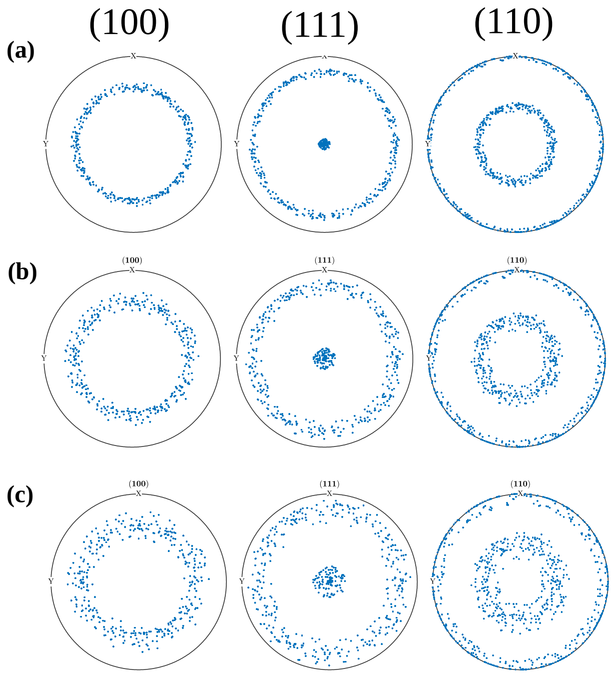
Ju X, Moumni Z, Zhang Y, et al. International Journal of Plasticity, 2022.

Results

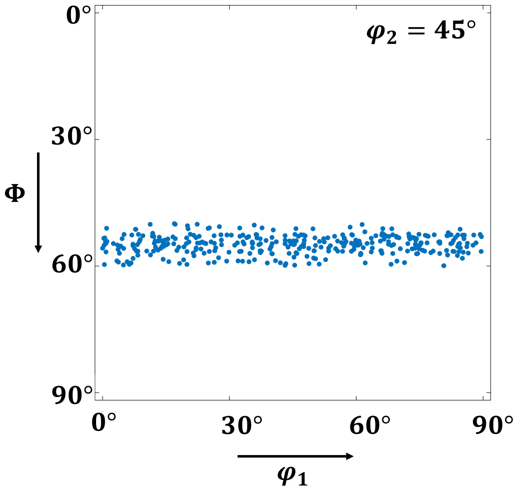
Polycrystalline



[111] // RD



[111] // ND



Random Orientation