Numerical modeling
that predicts, optimizes and innovates

Numerical Characterizations of Viscoplastic Behavior of TA6V with Metallurgical Phase Change

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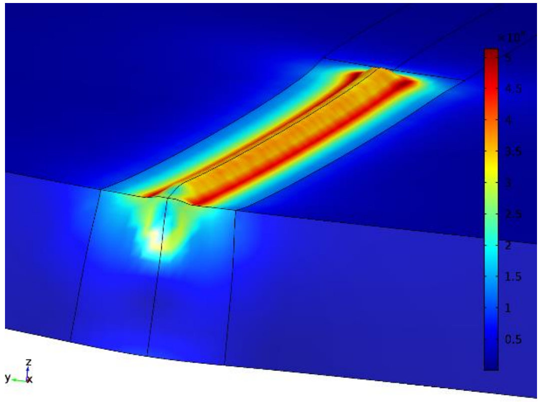

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SIMTEC, www.simtecsolution.fr

COMSOL Certified Consultant

- French company, founded in 2006, 4 Ph. D. Engineers
- Experts in Modeling, COMSOL Certified Consultants:
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  - Structural mechanics
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  - Heat transfer
  - Chemical engineering
- Services:
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  - Modeling assistance
- Main Clients:

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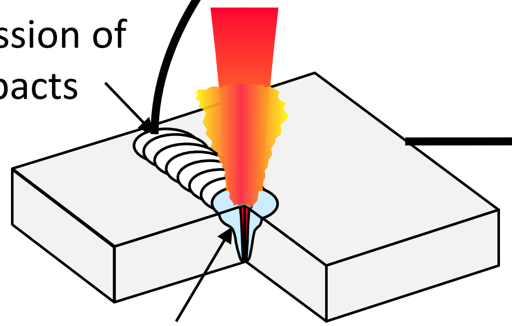
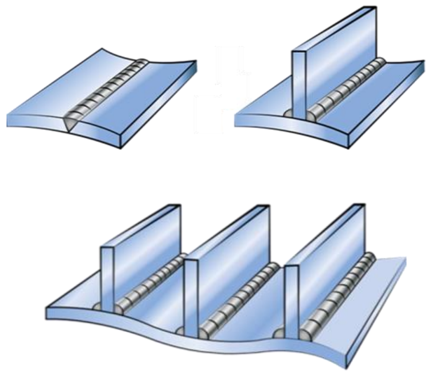
Problem / Objectives

Pulsed Laser Welding



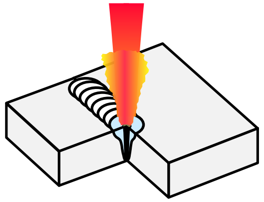
- **Highly localized heating**
- **Phase transitions**
- **Non-uniform** dilatation and contraction of the material



To predict the **residual stresses** and **distortions** after welding in order to **optimize the process**

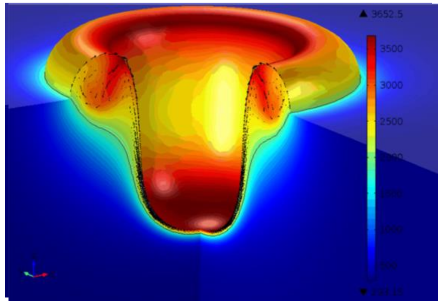
COMSOL

Physical Phenomena



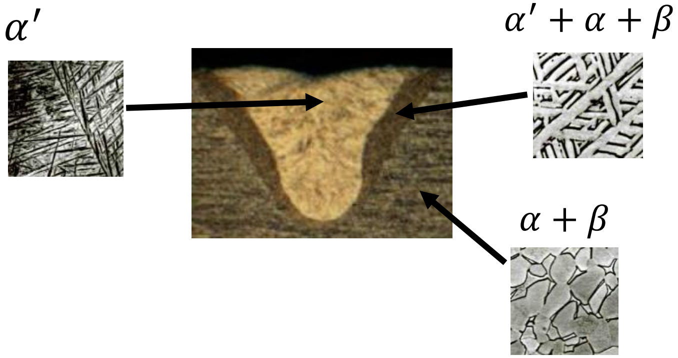
Thermo-hydraulic

- Laser/matter interaction
- Welding pool formation



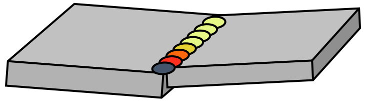
Thermo-metallurgy

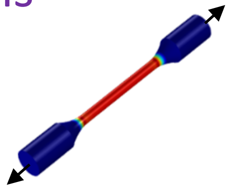
- Metallurgical phase changes



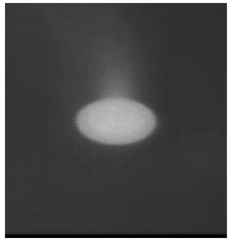
Thermo-mechanics

- Residual stresses
- Plastic deformations



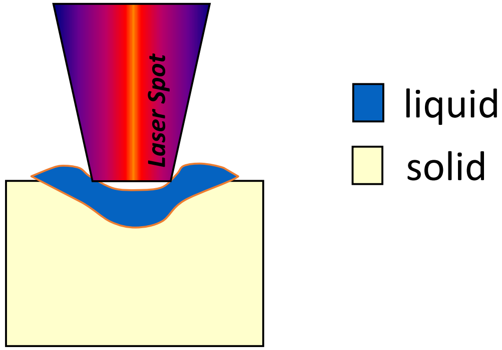


Thermo-hydraulic Phenomena



From

Vaporization process



- **Recoil pressure** generation induced by the **vaporization process**
- **Deformation of the vapor/liquid interface**

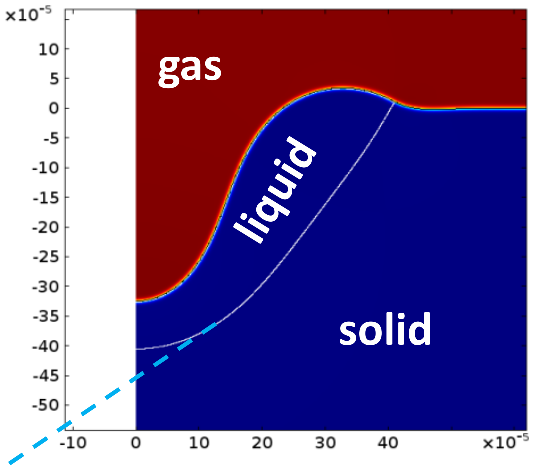
- "Keyhole" formation
- Increase of the global absorptivity

2 thermodynamic phase transitions:

fusion and **vaporization**

Thermo-hydraulic Model

- A three-phase description:
  - **Two-Phase Flow, Phase Field approach**



Bruyere et al. A Phase Field Approach to Model Laser Power Control in Spot Laser Welding, *Proceedings of the 2014 Comsol Conference Cambridge* (2014)

- Melting Transition:

Heat transfer

In condensed phase:

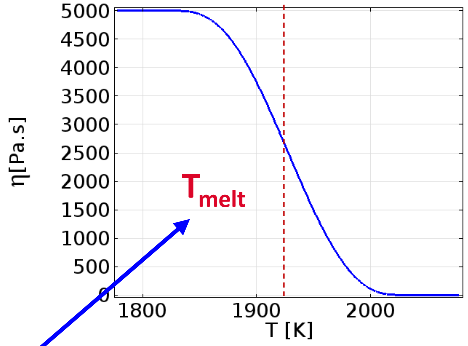
$$\rho C_p \frac{\partial T}{\partial t} + \rho C_p \boldsymbol{u} \cdot \nabla T = \nabla \cdot (k \nabla T) + Q_i$$

$$\begin{cases} \rho = \rho(T) \\ C_p = C_p(T) + L_f \dfrac{d\alpha}{dT} \quad \text{with } \displaystyle\int_{T_{melt}-\frac{\Delta T}{2}}^{T_{melt}+\frac{\Delta T}{2}} \frac{d\alpha}{dT} dT = 1 \\ k = k(T) \end{cases}$$

$$\Delta T = 40K$$
$$L_f = 3{,}9 \cdot 10^5\ J/kg$$

CFD

Viscosity evolution



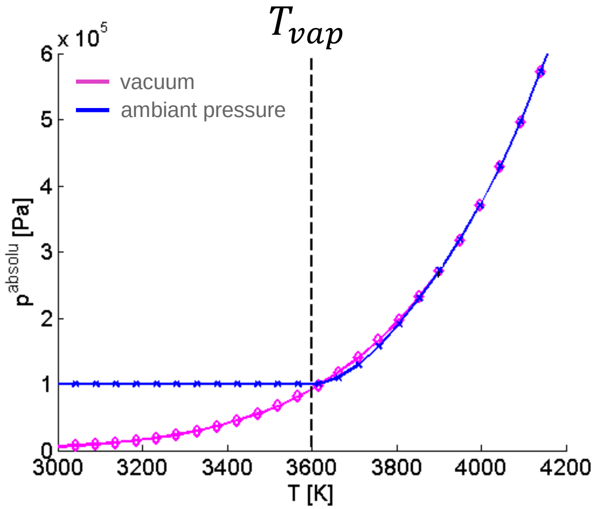
$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \boldsymbol{u} = 0$$

$$\rho \frac{\partial \boldsymbol{u}}{\partial t} + \rho(\boldsymbol{u} \cdot \nabla)\boldsymbol{u} = \nabla \cdot \left[-p\bar{\bar{I}} + \eta(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T)\right] + \rho \boldsymbol{g} \beta (T - T_{melt})$$

Vaporization Process

- **CFD:** Recoil pressure generation
  - Mass transfer neglected
  - Pressure jump added at the liquid/gas interface when $T > T_{vap}$

$$p_{sat}^{Clapeyron} = p_0 e^{\frac{L_v M^{mol}}{R^{mol} T_{vap}}\left(1-\frac{T_{vap}}{T}\right)}$$

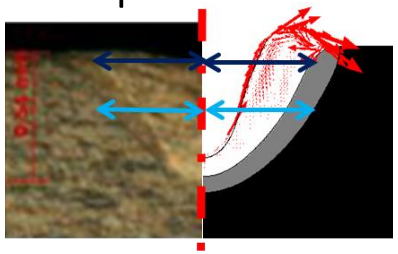


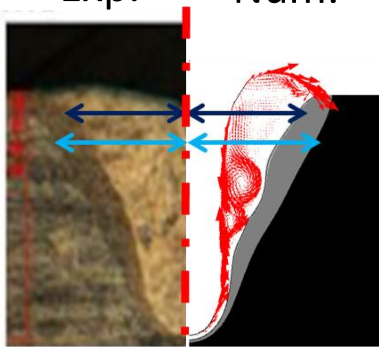
- **Heat transfer:** Vaporization flux

$$\dot{m} = (1-\beta_R)\sqrt{\frac{M^{mol}}{2\pi R^{mol} T}}\,(p_{sat}^{Clapeyron} - p_{amb})$$

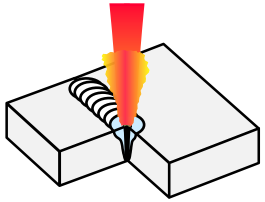
$$Flux_{vap} = -L_v \cdot \dot{m}$$

Results:





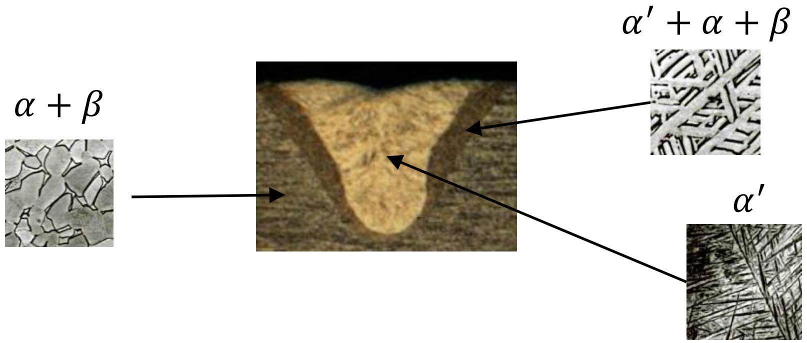
Metallurgical Behavior and Modeling



TA6V (90% Titanium, 6% Aluminum, 4% Vanadium)

3 metallurgical phases: α, α', β

- At initial state, $T = 20°C$, $z_\alpha = 92\%$, $z_{\alpha'} = 0$, $z_\beta = 8\%$
- During the heating process, a **metallurgical phase change** occurs if $T > T_{beta}$, $z_\beta \nearrow$ $z_\alpha \searrow$
- During the cooling process, the β-phase is partially or totally transformed into α'-phase



⇨ 2 ODEs

α-phase:

$$\dot{z_\alpha} = \begin{cases} z_\alpha * \dfrac{z_{max}^c(T) - z_\alpha - z_{\alpha'}}{\tau_\alpha(T)} & if\ (T < T_\beta) \\ z_\alpha * \dfrac{z_{max}^h(T) - z_\alpha - z_{\alpha'}}{\tau_\alpha(T)} & if\ (T > T_\beta) \end{cases}$$

α'-phase:

$$\dot{z_{\alpha'}} = \begin{cases} z_{\alpha'} * \dfrac{z_{max}^c(T) - z_\alpha - z_{\alpha'}}{\tau_{\alpha'}(T)} & if\ (\dot{T} > 0) \\ -\dfrac{z_\beta}{\tau_B(T)}\dot{T} & if\ (\dot{T} < 0) \end{cases}$$

β-phase:

$$z_\beta = 1 - z_\alpha - z_{\alpha'}$$

⇨ Coefficients calibrated with literature data

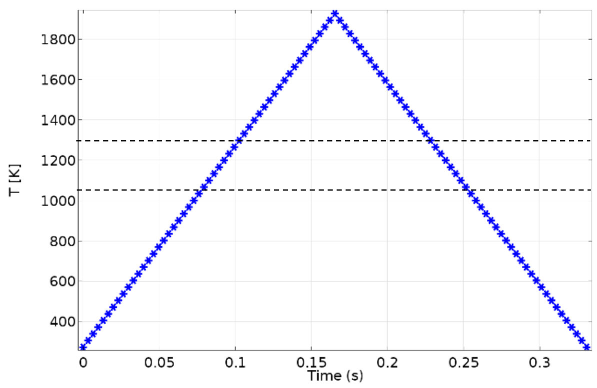
Y. Robert, « *Simulation numérique du soudage du TA6V par laser YAG impulsionnel : caractérisation expérimentale et modélisation des aspects thermomécanique associées à ce procédé* », PhD, « Ecole des mines de Paris », 2007

Metallurgical COMSOL Model

- 0D-model in COMSOL (**2 point ODEs**)

$$\frac{dT}{dt} = 10\,000[K/s]$$

Temperature cycle [K]

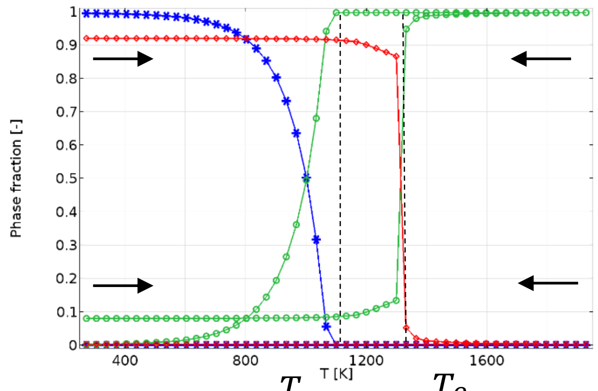


T_{melt}

T_{β}

T_m

Phase fraction [-]



T_m T_{β}

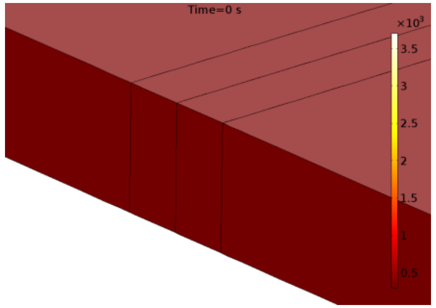
$$\dot{z_{\alpha}} = f(z_{\alpha}, z_{\alpha'}, T, \dot{T})$$

$$\dot{z_{\alpha'}} = f(z_{\alpha}, z_{\alpha'}, T, \dot{T})$$

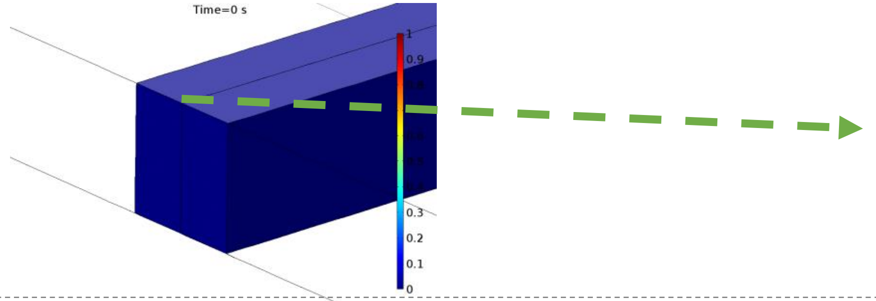
$$z_{\beta} = 1 - z_{\alpha} - z_{\alpha'}$$

- 3D example with welding operating conditions (**2 domain ODEs**)

T [K]

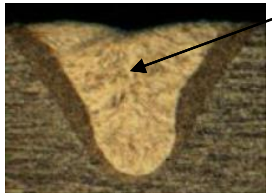


$z_{\alpha'}$ [-]

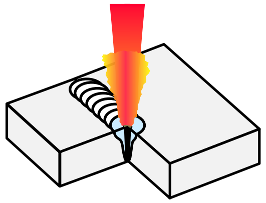


Experimental Fusion Zone after cooling

$z_{\alpha'} = 1$



Mechanical Behavior and Modeling



From literature [1,2]:

- Influence of **viscoplastic effects** at **high temperature** $\left(T > 0{,}5 * T_{fusion}\right)$
- Predominance of Baushinger effect → **kinematic hardening**
- **No isotropic hardening**

$$\underline{\underline{\varepsilon}} = \underline{\underline{\varepsilon}}^e + \underline{\underline{\varepsilon}}^p$$

$$\underline{\underline{\sigma}} = \underline{\underline{\underline{\underline{\mathbb{E}}}}}(T) : \left(\underline{\underline{\varepsilon}} - \underline{\underline{\varepsilon}}^p - \alpha(T, z_i) \cdot (T - T_0)\underline{\underline{\boldsymbol{I}}}\right)$$

Viscoplasticity with non-linear kinematic hardening

Thermal Dilatation

$$\dot{\underline{\underline{\varepsilon}}}^p = \dot{p}\,\frac{3}{2}\,\frac{\underline{\underline{\sigma}}' - \underline{\underline{X}}'}{J_2\left(\underline{\underline{\sigma}}' - \underline{\underline{X}}'\right)}$$

$$\dot{\underline{\underline{X}}} = \frac{2}{3} C(T)\dot{\underline{\underline{\varepsilon}}}^p - \gamma \underline{\underline{X}}\,\dot{p}$$

$$\dot{p} = \left\langle \frac{J_2\left(\underline{\underline{\sigma}} - \underline{\underline{X}}\right) - \sigma_y(T)}{K(T)} \right\rangle^{\mathrm{n(T)}}$$

"Lemaître & Chaboche" model

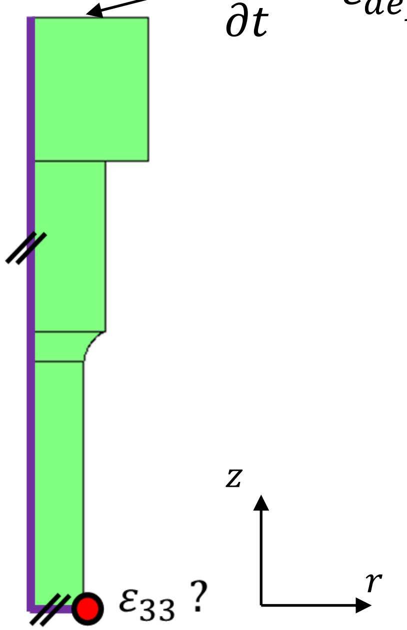
↓

3D :
13 domain ODEs

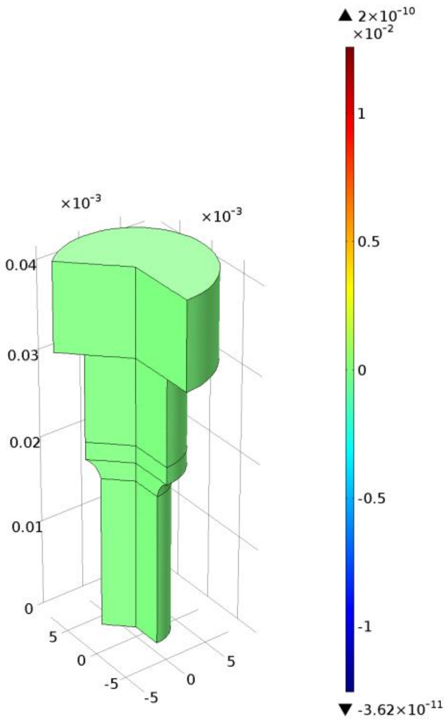
Mechanical COMSOL Model

- 2D-axi model

$$\frac{\partial w}{\partial t} = \dot{\varepsilon}_{def} L_0 \cdot f(t)$$



+ constraint : $|\varepsilon_{33}| \leq 0{,}01$



*Deformation scale * 50*

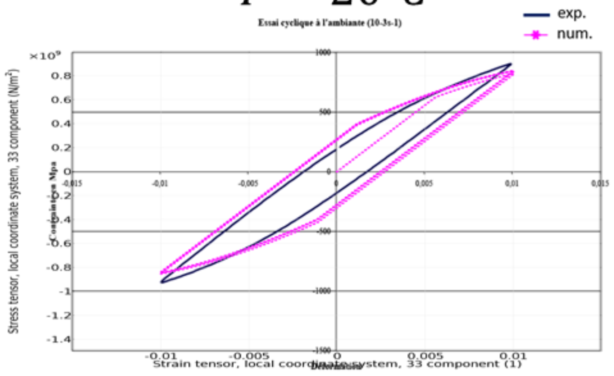
- $\dot{\varepsilon}_{def} = 10^{-3} s^{-1}$
- 6 temperatures :
  $T_0 = [20, 200, 400, 500, 600, ,800]\ \{°C\}$
- Mechanical coefficients obtained from literature and computations

Y. Robert, « *Simulation numérique du soudage du TA6V par laser YAG impulsionnel : caractérisation expérimentale et modélisation des aspects thermomécanique associées à ce procédé* », PhD, « Ecole des mines de Paris », 2007

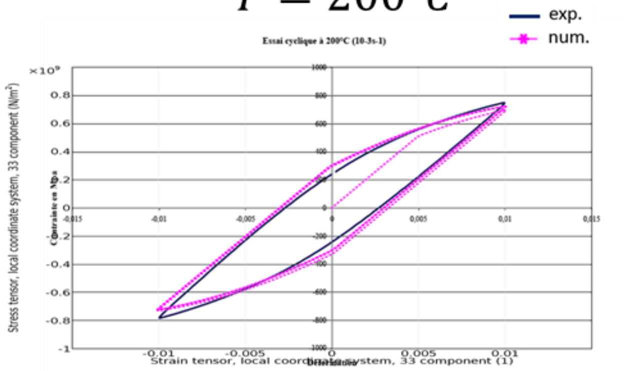
Thermo-mechanical Results

Comparison with experimental results (from Robert)

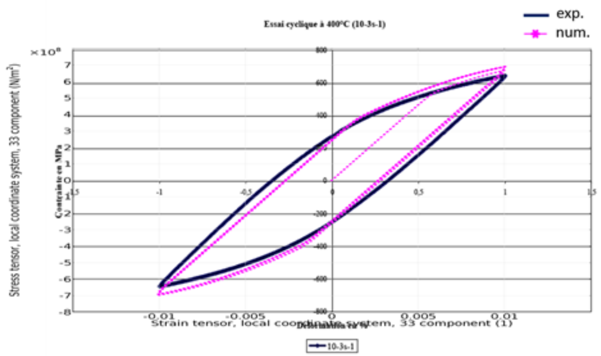
$T = 20°C$



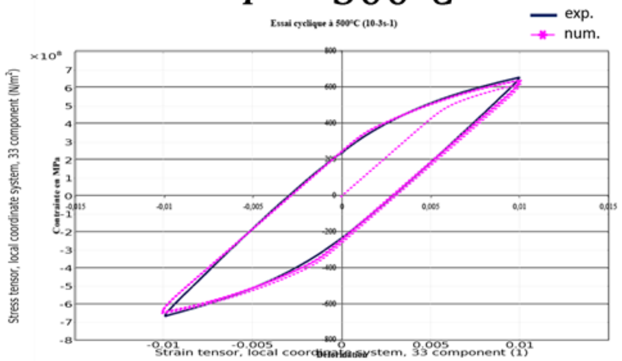
$T = 200°C$



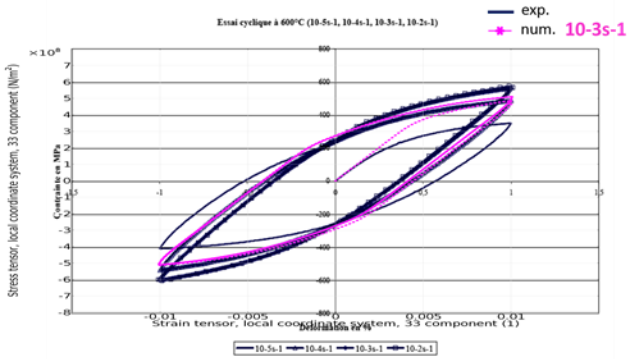
$T = 400°C$



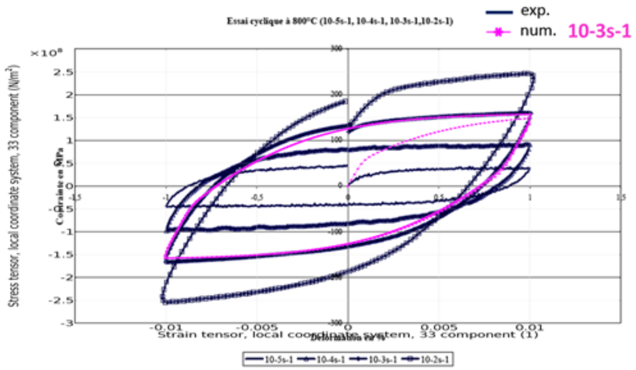
$T = 500°C$



$T = 600°C$

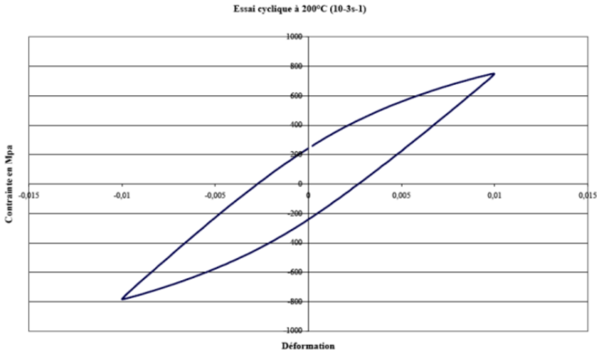
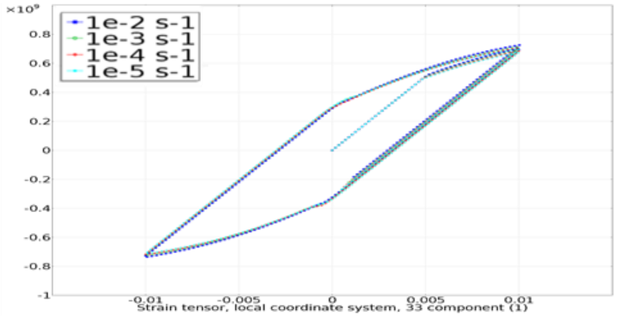
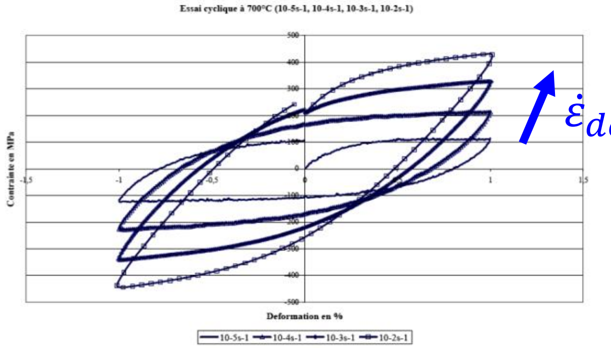
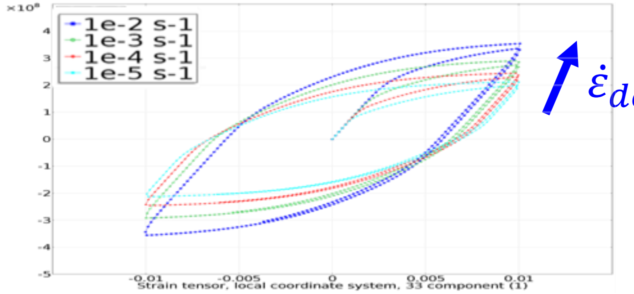


$T = 800°C$



Experimental Characterization

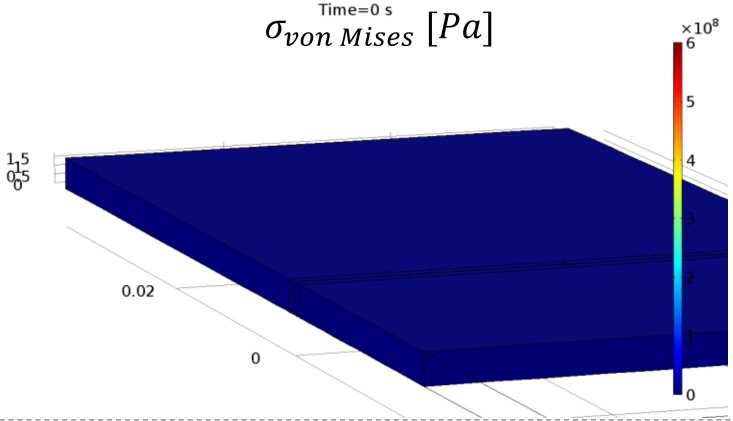
Influence of the deformation rate

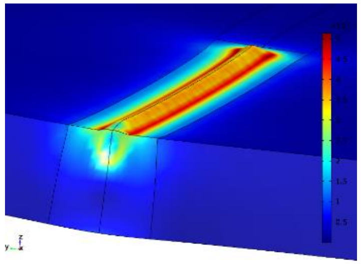
	Experimental	*Numerical*	
$T_0 = 200°C$			**No influence**
$T_0 = 700°C$	 $\dot{\varepsilon}_{def}$	 $\dot{\varepsilon}_{def}$	**Influence** of viscoplastic effects

Conclusions and Outlooks

- **Fusion** and **vaporization phase changes** modeled with COMSOL
- Development of a **thermo-mechanical** model taking into account:
  - **metallurgical phase change**
  - **non-linear kinematic hardening**
  - **viscoplastic effects**
- **Validation** of the numerical implementation in COMSOL by **comparison with experimental results**

Relevant for **industrial operating conditions** such as pulsed laser welding





Thanks for your attention .. and your questions!

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