Modelling of phase transformation in titanium alloy Ta6V Application to laser welding and laser prototyping

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1. Presentation of the industrial processes
2. Constitutive models
3. Validation

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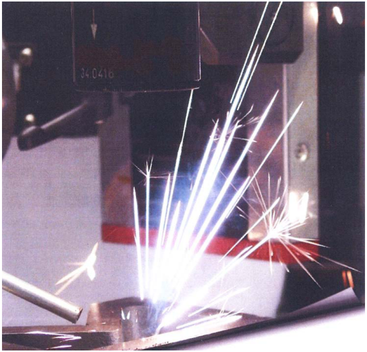
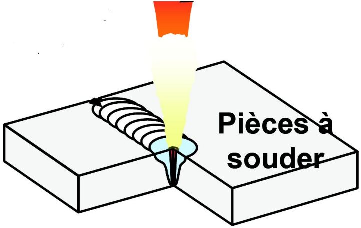
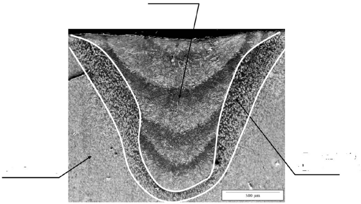
Laser welding (1/2)



- Tests performed at CEA Valduc(DFTN/SPAC/LSO)
- PhD student: Y. Robert
- Very precise welding
- No heating of the components
- Rapid welding cycles
- Work supported by CEA Valduc

Laser welding (2/2)

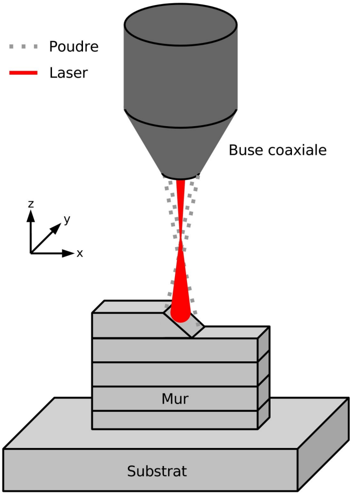


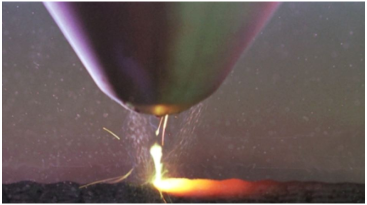


- Laser YaG
- Impulsion: 1–20 ms
- Frequency: 1–1000 Hz
- Mean power: 70–1500 W

- Keyhole development by heating–sublimation–plasma formation
- A given material point will melt several times
- Need for a good characterization of the residual stresses and component deformations

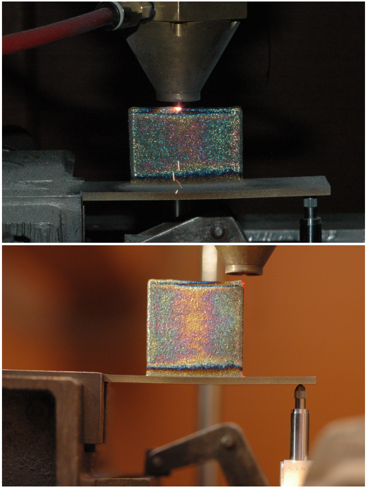
Laser prototyping (1/2)





- **Tests performed at French–German research center on lasers, CLFA (Arcueil, France)**
- **PhD student: A. Longuet**
- **Near the final shape**
- **Work supported by PROFIL consortium (french aeronautical industry)**

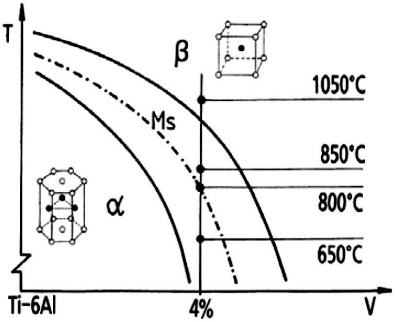
Laser prototyping (2/2)

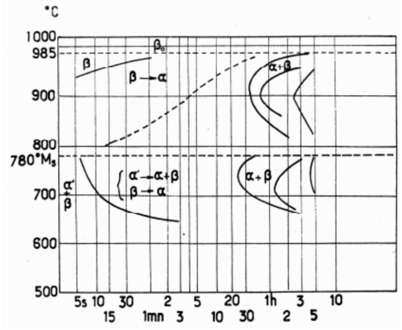


- **Power: 100–1000 W**
- **Speed: 100–500 mm/min**
- **Beam diameter: 1–3 mm**
- **Deposit height: 0.1–0.6 mm**

- **Construction of any complex shape**
- **Need for a good characterization of the residual stresses and component deformations**

Characteristic diagrams for Ta6V

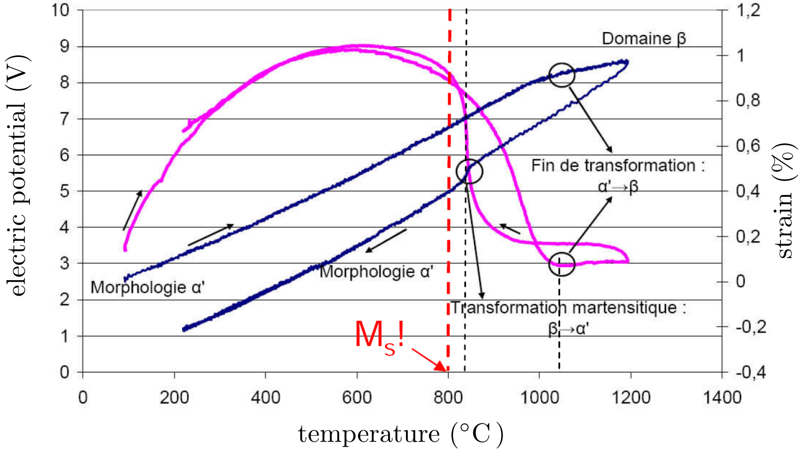




Pseudo-binary diagram
β stabilized by V
at low temperature

Time–temperature plots
(Hocheid, 1970)
Not fully characterized

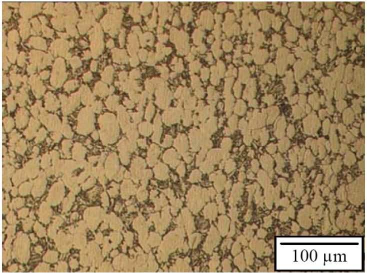
Dilatometry test (no charge)



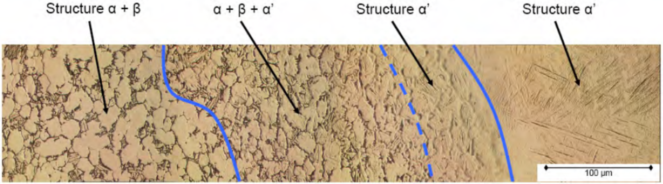
Drastical change of the resistivity

Typical microstructures in the welding problem

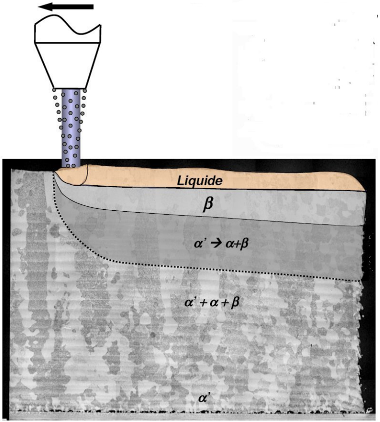
Base metal



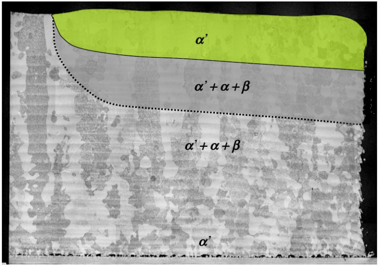
α' microstructure



Typical microstructures in the prototyping problem



Heating



Cooling

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Metallurgical model (1/2)

Phase	without Vanadium	with Vanadium
HCP	α	α'
CC	$\beta - \beta_t$	β_t

- **Equilibrium phases: α and β_t**
- **Evolution rules for the variables: z_α and $z_{\alpha'}$, z_{β_t}**
- **Amount of phase β: $z_\beta = 1 - z_\alpha - z_{\alpha'}$**
- **z_{β_t} is the amount of β phase that can be transformed into α'**
- **Different regimes according to $\dot{T}$ (cooling or heating): diffusion controlled transformation during heating and tempering, martensitic transformation during cooling**
- **Material parameters: $\mathbf{z}_\alpha^{max}$, the equilibrium volume fraction of $\alpha + \alpha'$ and time constants for each phase, τ_α, $\tau_{\alpha'}$, τ_β, τ_t**

Metallurgical model (2/2)

- **Heating** $\dot{T} \geqslant 0$

$$\dot{z}_\alpha = \frac{z_\alpha \left(\mathbf{z}_\alpha^{max} - z_\alpha - z_{\alpha'} \right)}{\tau_\alpha}$$

$$\dot{z}_{\alpha'} = \frac{z_{\alpha'} \left(\mathbf{z}_\alpha^{max} - z_\alpha - z_{\alpha'} \right)}{\tau_{\alpha'}}$$

- **Cooling** $\dot{T} < 0$ **and** $T < M_s$

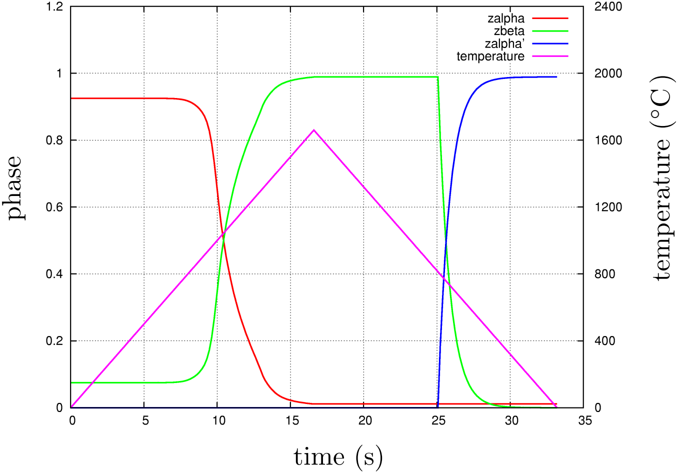
$$\dot{z}_{\alpha'} = -\frac{z_{\beta t}\,\dot{T}}{\tau_\beta}$$

- **For any** $\dot{T}$

$$\dot{z}_{\beta t} = \frac{z_\beta \left(z_\beta - z_{\beta t} \right)}{\tau_t}$$

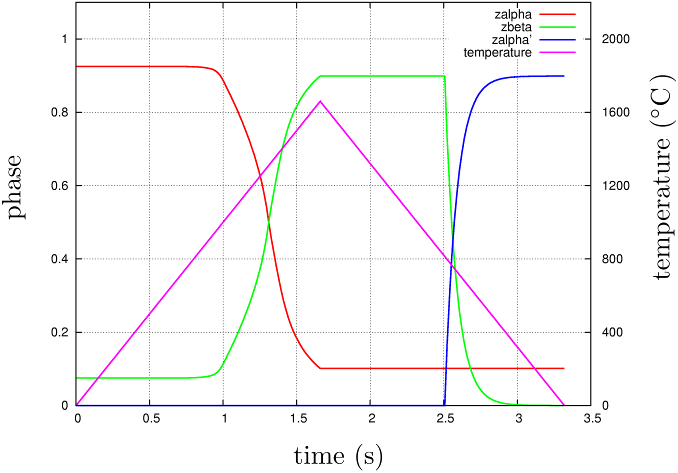
Typical behaviour of the phase transformation model

Start in α+β at RT, low $\dot{T}$, total transformation



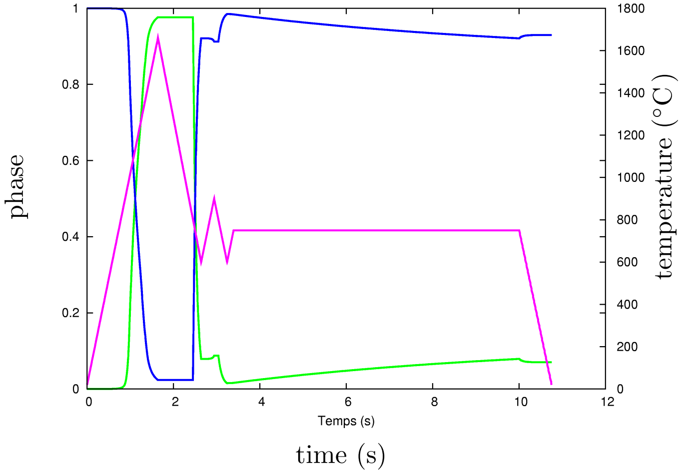
Typical behaviour of the phase transformation model

Start in $\alpha+\beta$ at RT, high $\dot{T}$, partial transformation

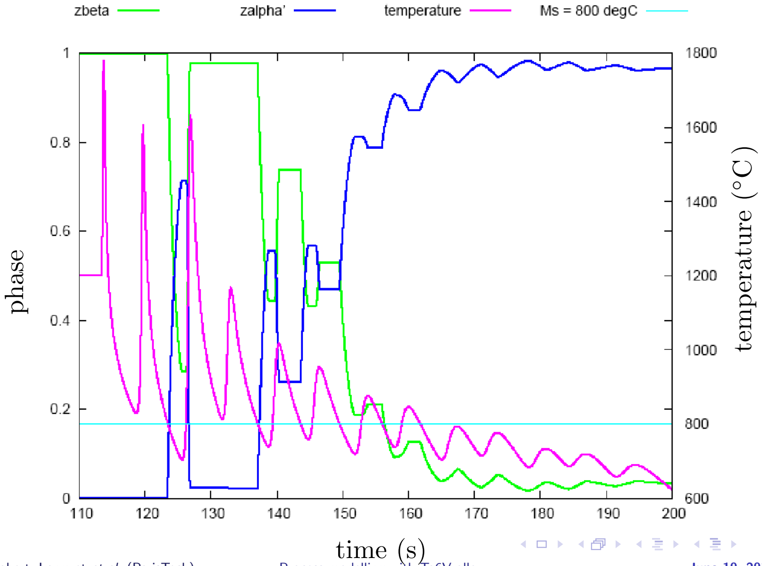


Typical behaviour of the phase transformation model

Start in pure α', cooling and TT, subsequent evolution



An example of temperature and phase history (prototyping)



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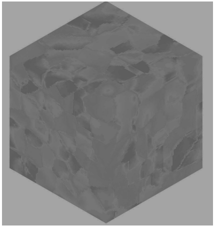
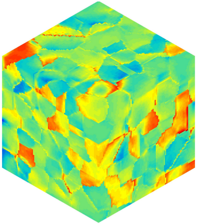
Mechanical modelling at various scales

Black box



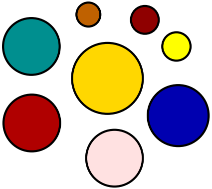
Level (1)
Macroscopic models
Average stress and strain tensor

Realistic aggregate



Level (3)
Local information
Respect local Constitutive Equations
Equilibrium

Uniform field



Level (2)
Local average
Respect local Constitutive Equations
no neighbouring effect

Remarks on the micro–macro modelling strategy

- **Step 1: Representation of the microstructure**
  - **Geometry, Phase contrast, texture**
  - **Is a "Phase" defined by its chemestry, crystal orientation, shape,. . . ?**
  - **Macro–Grains–Phases or Macro–Phases ?**
- **Step 2: Characterization of the local behaviour**
  - **Can we generate isolated phases ?**
- **Step 3: Selection of a scale transition rule**
  - **Depending on the geometry,. . .**
- **HERE: 3 phases only**
  - **Grains, needles,. . . are not considered independently, but the information is collected into an unique "phase"**
  - **Elasticity and thermal dilatation properties are supposed to be homogeneous**
  - **Volumetric change due to a different compacity of cubic and hexagonal phases**

Critical variables in the model

Using $\mathcal{I}$ to denote the phase set, $l \in \mathcal{I} = \{\alpha, \alpha', \beta\}$

	Variables	Volume fraction
Macro scale	$\underset{\sim}{\sigma}$, $\underset{\sim}{\varepsilon}^p$	1
Phase scale	$\underset{\sim}{\sigma}^\alpha$, $\underset{\sim}{\sigma}^{\alpha'}$, $\underset{\sim}{\sigma}^\beta$	z^l
	$\underset{\sim}{\varepsilon}^\alpha$, $\underset{\sim}{\varepsilon}^{\alpha'}$, $\underset{\sim}{\varepsilon}^\beta$	$\sum_{l \in \mathcal{I}} z^l = 1$

- **Three plastic deformation mechanisms are considered, in phases α, α', β**
- **A model with isotropic and kinematic hardening, depending on local stress, introducing one yield function for each phase**

$$f^l(\underset{\sim}{\sigma}^l, \underset{\sim}{\mathbf{X}}^l, R^l) = J(\underset{\sim}{\sigma}^l - \underset{\sim}{\mathbf{X}}^l) - R^l - \mathbf{R}_l^0$$

- **Three tensors and three scalars: $\underset{\sim}{\mathbf{X}}^\alpha$, $\underset{\sim}{\mathbf{X}}^{\alpha'}$, $\underset{\sim}{\mathbf{X}}^\beta$, R^α, $R^{\alpha'}$, R^β as hardening variables**

Constitutive equations in each phase

- **Computation of the macroscopic plastic strain**

$$\dot{\underset{\sim}{\varepsilon}}^p = \sum_{I \in \mathcal{I}} z^I \dot{\underset{\sim}{\varepsilon}}^I = z^\alpha \dot{\underset{\sim}{\varepsilon}}^\alpha + z^{\alpha'} \dot{\underset{\sim}{\varepsilon}}^{\alpha'} + (1 - z^\alpha - z^{\alpha'}) \dot{\underset{\sim}{\varepsilon}}^\beta$$

- **Computation of the local plastic strain rate as a function of the equivalent stress**

$$\dot{\underset{\sim}{\varepsilon}}^I = \left\langle \frac{f^I}{\mathbf{K}_I} \right\rangle^{\mathbf{n}_I} \frac{\partial f^I}{\partial \underset{\sim}{\boldsymbol{\sigma}}^I} = \dot{v}^I \underset{\sim}{\mathbf{n}}^I$$

- **Isotropic hardening, R^I function of r^I, such as**

$$R^I = \mathbf{b}_I \mathbf{Q}_I r^i \qquad \dot{r}^I = (1 - \mathbf{b}_I r^I) \dot{v}^I - \left(\frac{|R^I|}{\mathbf{P}_I} \right)^{\mathbf{p}_I}$$

- **Kinematic hardening, x^s function of α^s, such as**

$$\underset{\sim}{\mathbf{X}}^I = \frac{2}{3} \mathbf{C}_I \underset{\sim}{\alpha}^I \qquad \dot{\underset{\sim}{\alpha}}^I = (\underset{\sim}{\mathbf{n}}^I - \frac{3\mathbf{D}_I}{2\mathbf{C}_I} \underset{\sim}{\mathbf{X}}^I) \dot{v}^I - \left(\frac{J(\underset{\sim}{\mathbf{X}}^I)}{\mathbf{M}_I} \right)^{\mathbf{m}_I} \frac{\underset{\sim}{\mathbf{X}}^I}{J(\underset{\sim}{\mathbf{X}}^I)}$$

Choice of a scale transition rule

- **Taylor, uniform plastic strain – too stiff**

$$\dot{\underset{\sim}{\varepsilon}}^I = \dot{\underset{\sim}{\varepsilon}} \qquad \forall I \in \mathcal{I}$$

- **Uniform stress – too soft**

$$\underset{\sim}{\sigma}^I = \underset{\sim}{\sigma} \qquad \forall I \in \mathcal{I}$$

- **Kröner's elastic accommodation rule – too stiff**

$$\underset{\sim}{\sigma}^I = \underset{\sim}{\sigma} + \mu(\underset{\sim}{\varepsilon}^p - \underset{\sim}{\varepsilon}^I)$$

- **"Beta" rule, elastoplastic accommodation rule – continuous evolution**

$$\underset{\sim}{\sigma}^I = \underset{\sim}{\sigma} + \mathbf{C}(\underset{\sim}{\beta} - \underset{\sim}{\beta}^I)$$

$$\dot{\beta}^I = \dot{\underset{\sim}{\varepsilon}}^g - \mathbf{D}\underset{\sim}{\beta}^g \parallel \dot{\underset{\sim}{\varepsilon}}^g \parallel \qquad \underset{\sim}{\beta} = \sum_{I \in \mathcal{I}} z^I \underset{\sim}{\beta}^I$$

Summary of the independent variables and material parameters

Variable type	Name	Nature	# scalars
Elastic strain	$\underset{\sim}{\varepsilon}^e$	1 tensor	6
Macro. to phase	$\underset{\sim}{\beta}^I$	3 tensors	18
Kin. hard. in phases	$\underset{\sim}{\alpha}^I$	3 tensors	18
Iso. hard. in phases	p^I	3 scalars	3
Phase vol. fractions	z^{α}, $z^{\alpha'}$, $z^{\beta t}$	3 scalars	3
Total	....	....	48

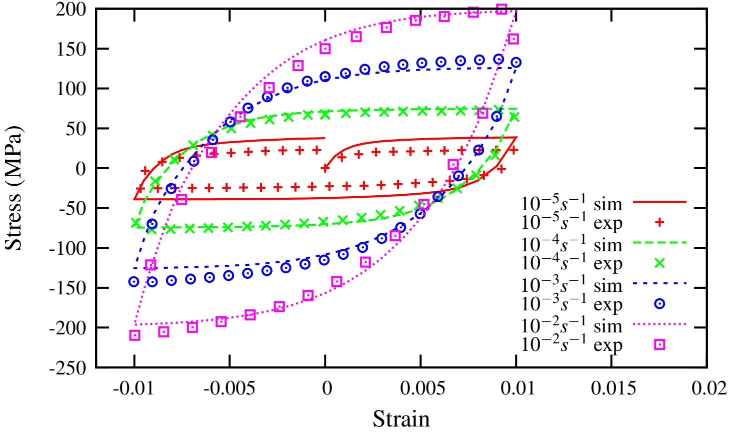
Parameter type	Name	# scalars
Viscosity in phase	$\mathbf{K}_I$, $\mathbf{n}_I$	6
Iso. hard. in phases w. recov.	$\mathbf{Q}_I$, $\mathbf{b}_I$, $\mathbf{R}_I^0$, $\mathbf{P}_I$, $\mathbf{p}_I$	15
Kin. hard. in phases w. recov.	$\mathbf{C}_I$, $\mathbf{D}_I$, $\mathbf{M}_I$, $\mathbf{m}_I$	12
Scale transition rules	**C**, **D**	2
Metallurgical model	$\mathbf{z}_{\alpha}^{max}$, τ_{α}, $\tau_{\alpha'}$, τ_{β}, τ_t	5
Total	....	40

Identification strategy

- **Sequential calculation , the influence of plastic deformation and phase change on temperature fields is negligeable**
- **An unique code,**

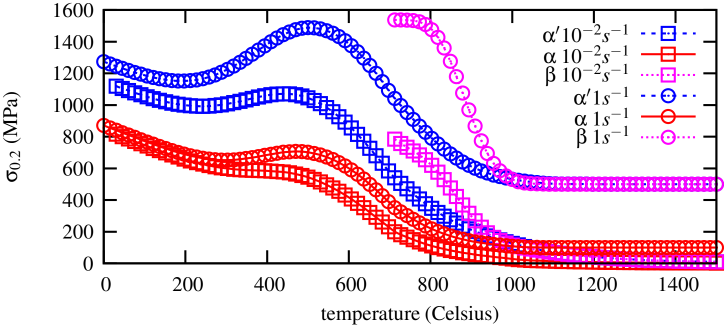
  `ZMaT` **, to implement the metallurgy+mechanics model – the same is used for identification and subsequent FE computations**
- **Need for a large data base , from RT to melting temperature, cyclic, with various phase contents**
- **Various TT are applied to specimens before the test starts**

Simulation of several cyclic tests at 800°C



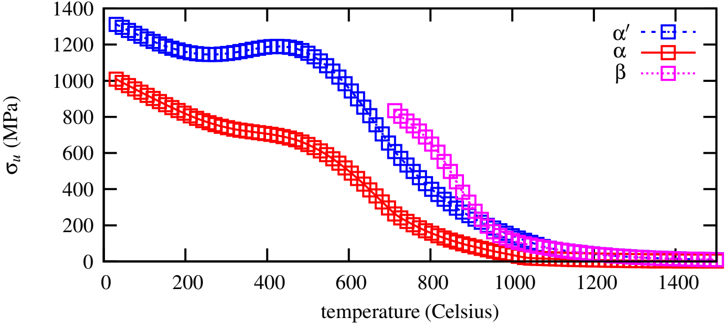
Large influence of the strain rate

Simulation of the yield stress



The viscous effect is phase dependent

Simulation of the ultimate stress



No significant stress level for $T > 1000^\circ$C

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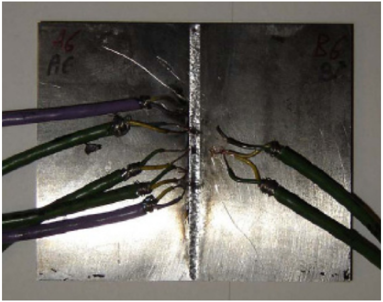
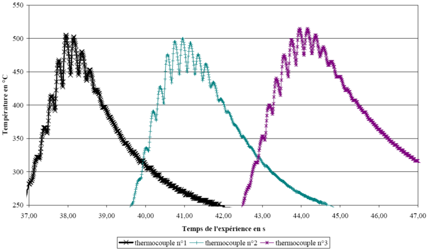
Welding of two plates





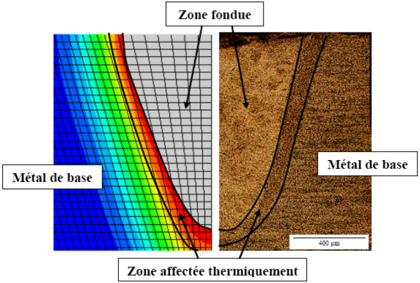
50 mm $\times$ 25 mm plates equipped with thermocouples

Temperature history for three thermocouples

Specimen and temperature histories

Specimen and temperature histories

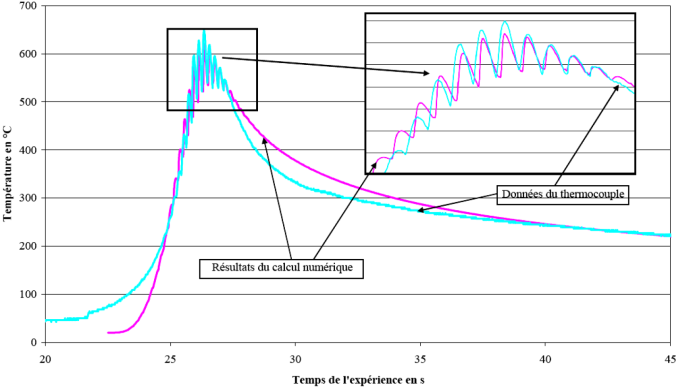
Plates with thermocouples



- Calibration of the simulated Heat Affected Zone (HAZ): Base metal, ZAT, melted zone

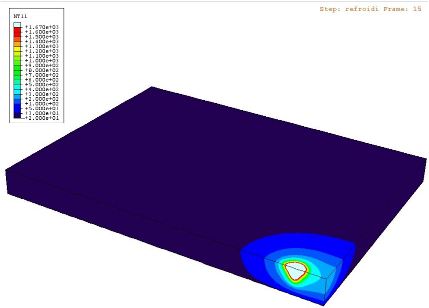
- 3D calculation performed with Abaqus (53064 nodes, min element size: 0.3 mm)
- Heat coming from the laser beam is modelled by a convection BC, according to a given geometry
- Heat loss by convection and radiation
- 123 laser implusions, period 200 ms (13 ms+187 ms)

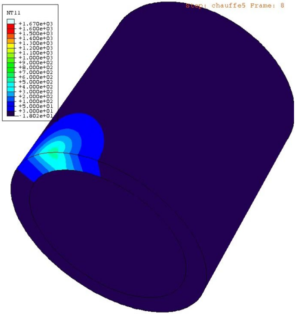
Comparison between simulation and experiments



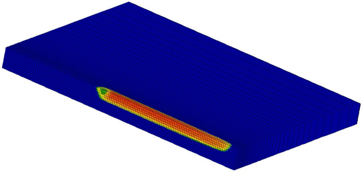
Temperature versus time

Thermal calculations during laser welding

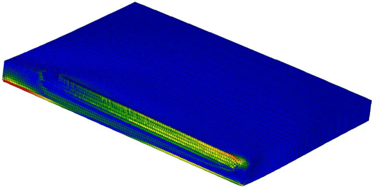




Simulation results



Amount of α'



Von Mises equivalent stress

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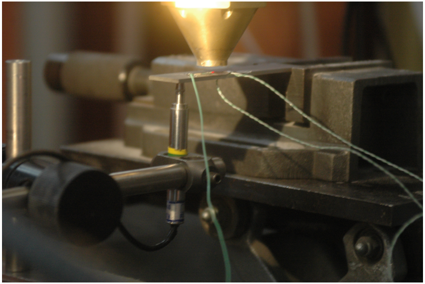
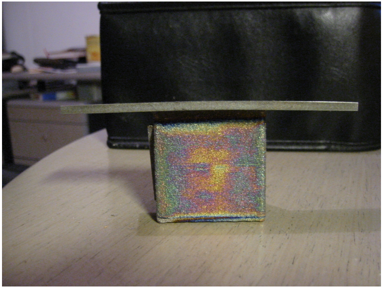
Validation test for laser prototyping

Fabrication of a "wall" on a substrate

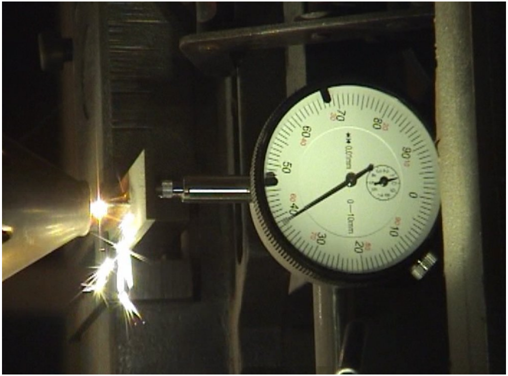


- Laser YaG
- Impulsion: 1–20 ms
- Frequency: 1–1000 Hz
- Mean power: 70–1500 W



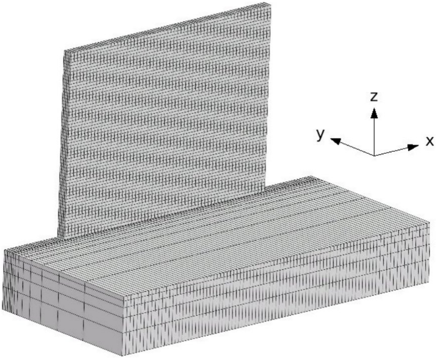
- Substrate 8 mm × 28 mm × 40 mm
- Length of the wall: 30 mm; width: 1.5 mm; 50 layers (20 mm)

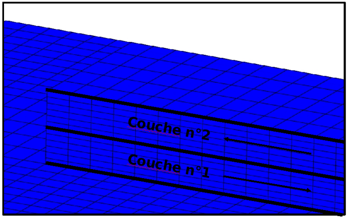
Deflection measurement during wall construction by laser prototyping

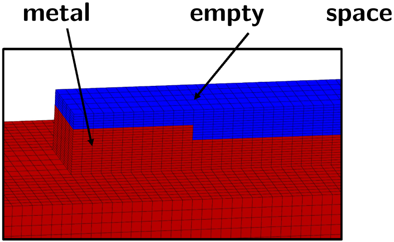


- **Dynamic measurement of the deflection during fabrication**
- **Discriminate between contributions of thermal expansion, elasticity, plasticity, phase transformation**
- **Provide a global sim–exp comparison**

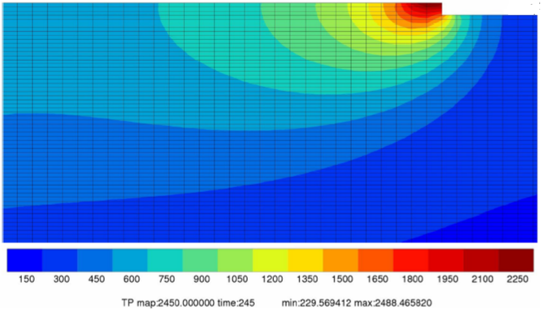
Mesh and element generation





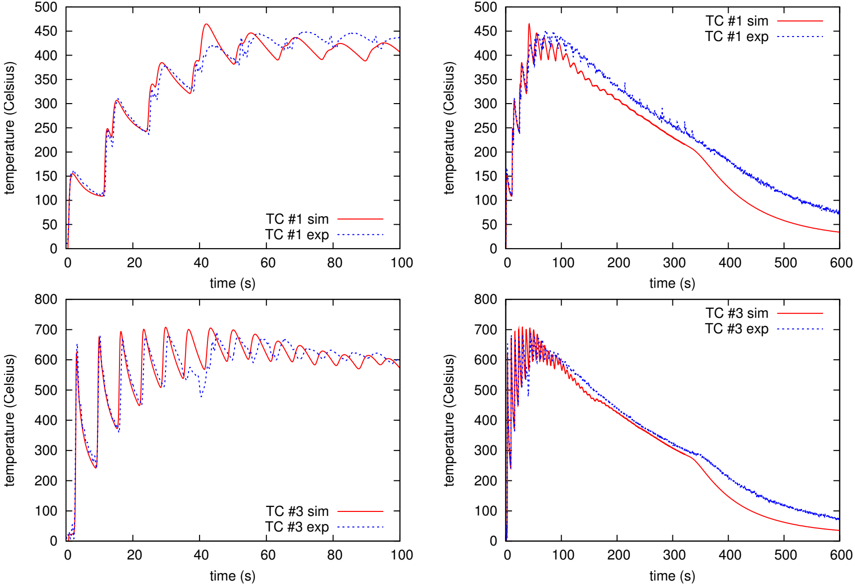


Thermal calculations during laser prototyping

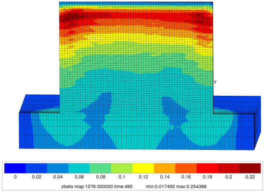


- FE analysis of the temperature field, code ZéBuLoN (100000 nodes, 3 elements/layer, 3 elements for half width)
- Moving boundary conditions
- Parabolic distribution of the heat flux inside the laser beam

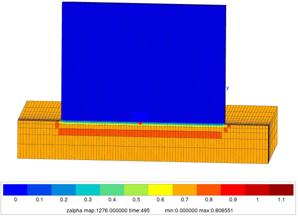
Temperature history for thermocouples 1 and 3



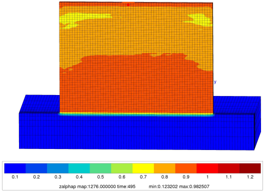
Simulation of the various phases at the end of the test



range: 0–0.20
phase β

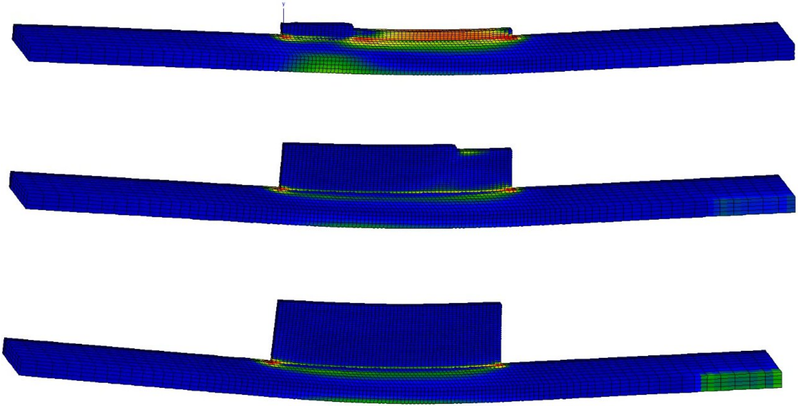


range: 0–0.80
phase α

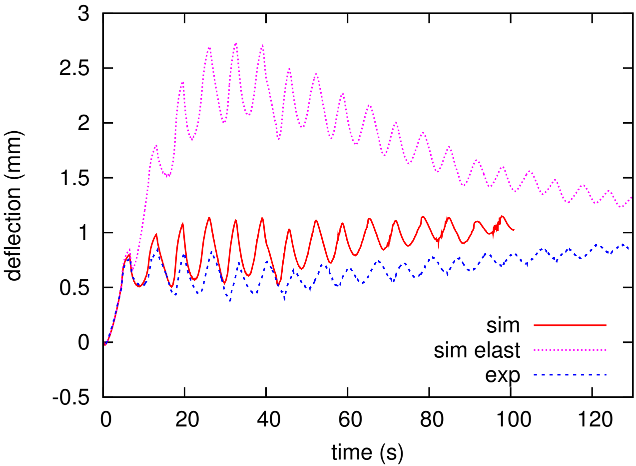


range: 0–1.00
phase α'

Mechanical calculations during laser prototyping



Evolution of the deflection during the fabrication



Nonlinear evaluation is mandatory

Conclusions and perspectives

- **Good prediction of the phases**
- **Good prediction of the residual stresses (not shown here)**
- **Rather good prediction of the deflection**
  - **welding test: exp, 0.28 mm – sim, 0.20 mm**
  - **prototyping test: exp:1.2 mm – sim, 1.0 mm**
- **A certain class of micro–macro model is now manageable in industrial FEA**
- **This is one element for a full prediction chain "from fabrication to destruction"**
- **The status obtained can be taken as the initial state of a structural calculation to determine the resistance of the componenent in operation**