LIÈGE université
Urban & Environmental Engineering

LIÈGE université

Prediction of Phase-transformations of Ti6Al4V additively manufactured during Directed Energy Deposition

Seifallah Fetni, Jérôme T. Tchuindjang, Anne Mertens, Anne M. Habraken

Materials and Solid Mechanics, University of Liège, Liège, Belgium

Metallic Materials Science, University of Liège, Liège, Belgium

18th European Mechanics of Materials Conference

Oxford 4th April 2022

Contents

Background & motivations

- Directed Energy Deposition
- TA6V

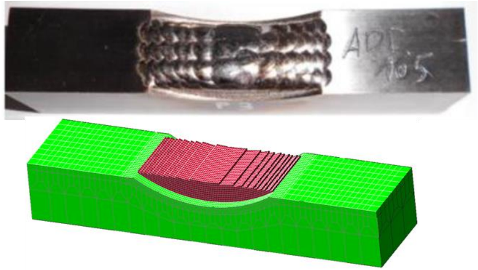
Implemented Models

- Finite Element Modeling
- TTB segmentation

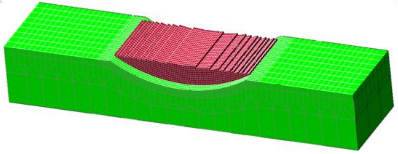
Machine Learning Framework

- Actual achievements
- TA6V Encoding and classification
- Proposed Framework

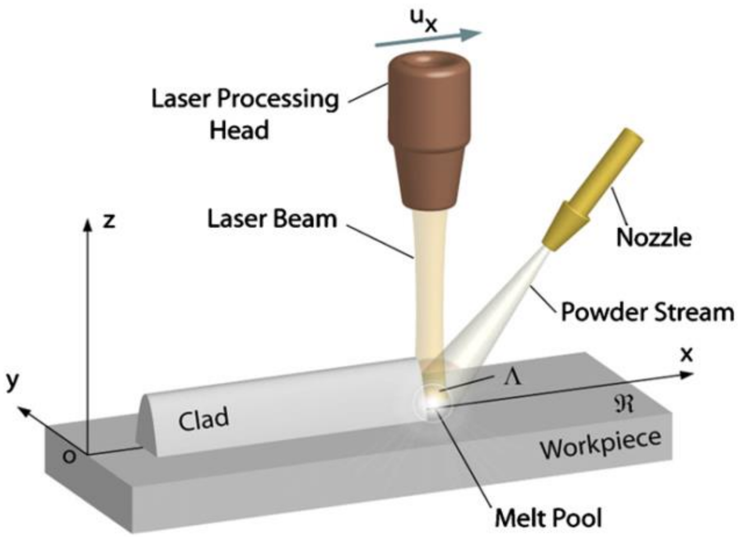
Conclusions

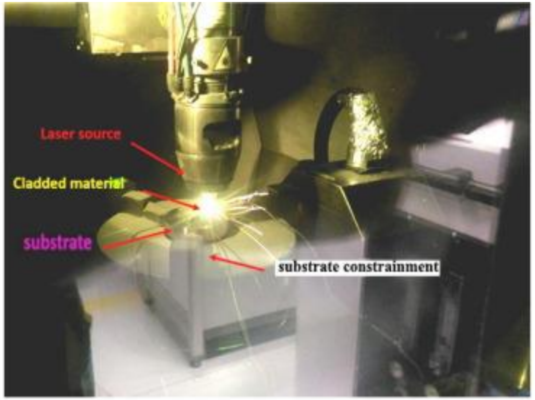


Contents

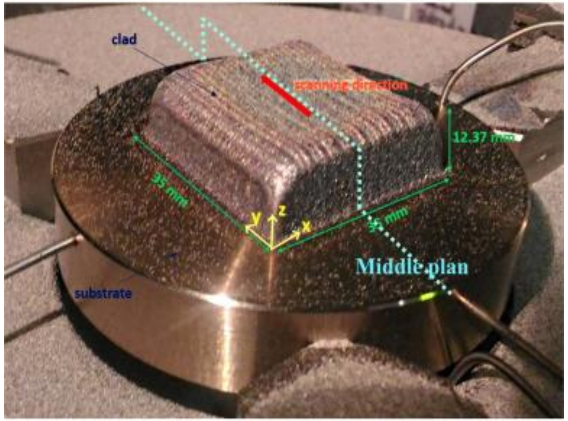


Background & motivations: *DED* Manufacturing





(a)



(b)

Input Laser High energy density ➔ each layer exhibits a thermal sequence {*1st cooling, reheating, 2nd cooling…*} ➔ *Heterogeneous* microstructure

S. Fetni, T. M. Enrici, T. Niccolini, H. S. Tran, O. Dedry, L. Duchêne, A. Mertens, A. M. Habraken, Thermal model for the directed energy deposition of composite coatings of 316L stainless steel enriched with tungsten carbides, Materials & Design, Volume 204, 2021,

Background & motivations: DED Manufacturing

EXPERIMENTAL ANALYSIS:

- **not completely exhaustive**
- **very expensive**

- ❑ **Out-of-equilibrium phases**
- ❑ **Typical AM microstructure**

=> Need for ***modeling*** to avoid cost-consuming trials and error experiments.

⇒ Validated **Numerical models** can deal with this issue.

⇒ **Accurate predictions** (thermal, thermo-mechanical, thermo-mechanical- metallurgical)

⇒ Knowledge of the thermal history ➔ nature and grain size of the phases.

⇒ Capabilities of *Machine Learning* techniques to learn Additively manufactured materials behaviors.

Contents

Background & motivations

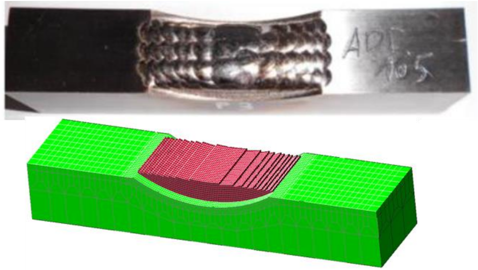
- Directed Energy Deposition
- TA6V

Implemented Models

- FEM model
- TTB segmentation

Machine Learning Framework

- Team Achievements
- Proposed Framework
- Encoding and classification



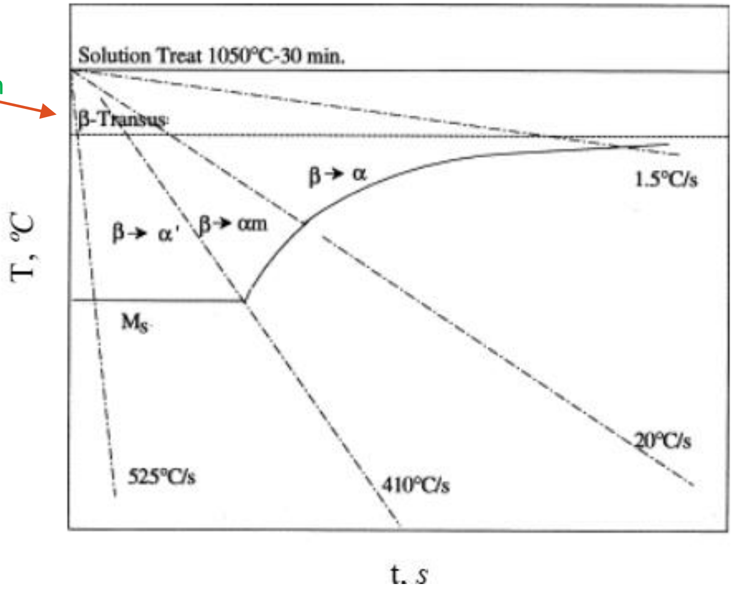
Conclusions

Ti6Al4V : Phases

Schematic continuous cooling diagram for Ti6Al4V

.

Temp of transition



- Cooling Rate (CR) after heat treatment (post-DED fabrication)
- The cooling rate enhances the genesis of the microstructure
- Reheating: heating transferred as result of remelting

Phases in TiAl6V:
α ,α', α_m ,β

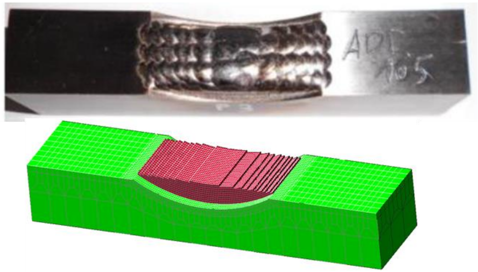
β ➔ α (or β_{ret}) : diffusional transformation (slow CR)

β ➔ α' : martensitic transformation (high CR)

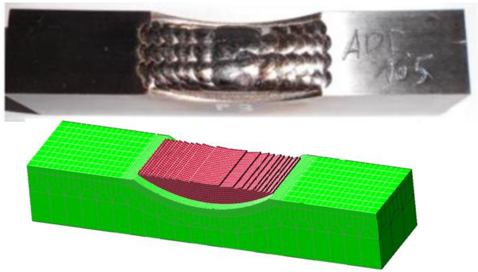
β ➔ α_m: massive

T. Ahmed and H. J. Rack, "Phase transformations during cooling in α+β titanium alloys," *Mater. Sci. Eng. A*, vol. 243, no. 1–2, pp. 206–211, 1998.

Contents



Contents



Finite Element Modeling of TiAl6V

Target: *Thermal Field* Predictions

Thermal equations

Heat transfer by conduction

$$\underbrace{\frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(k\frac{\partial T}{\partial y}\right)+\frac{\partial}{\partial z}\left(k\frac{\partial T}{\partial z}\right)}_{\text{Conductivity}}+Q_{\text{int}}=\rho c_p\frac{\partial T}{\partial t}$$

Density

Heat Capacity

Power gen. per volume (= 0)

→ **Lagamine** code

Heat transfer at boundary

- $k(\nabla T.n) = q_{laser} - h(T-T_0) - \varepsilon\sigma(T^4 - T_0^4)$

Laser Power   Convection Coef.   Emissivity

T : Temperature (K)
T_0 ambiance temperature
L : Liquidus
S: Solidus
L_f :Latent heat (solid-liquid)
h :convection
C_p :heat capacity
ε :radiation coef σ Boltzman constant

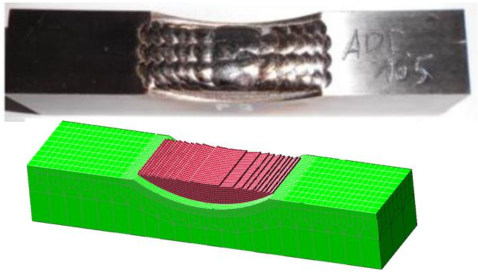
Latent heat of fusion

$$c_p^* = \frac{L_f}{T_L - T_S} + c_p$$

$$q_{laser} = \beta\, I(x,y,z,U,t)$$

Thermal field : better indications than residual stress state-based models ➔ achieve optimal parameters of *DED* processes

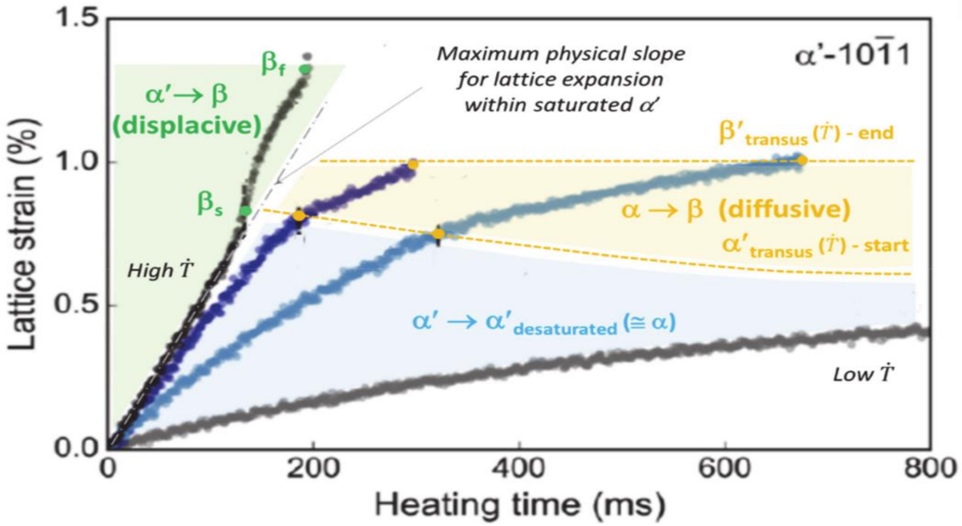
Contents



Introduction of TTB segmentation

- Segmentation of the temperature history in different blocks ➔ ***T**ime-phase* ***T**ransformation*-***B**lock*
- The transformations kinetics in TiAl6V are highly influenced by the reheating

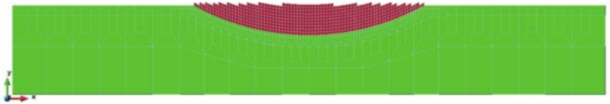
➔ Influence of heating rate $\dot{T}$ on the mechanism and transition points of the reverse transformations of α'

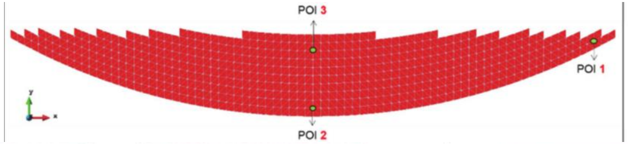


Kenel, C.; Grolimund, D.; Li, X.; Panepucci, E.; Samson, V.A.; Sanchez, D.F.; Marone, F.; Leinenbach, C. In situ investigation of phase transformations in Ti-6Al-4V under additive manufacturing conditions combining laser melting and high-speed micro-X-ray diffraction. Sci. Rep. 2017, 7, 16358

Introduction of TTB segmentation

Decreased track length ➔ Clad heterogeneity & graded microstructure

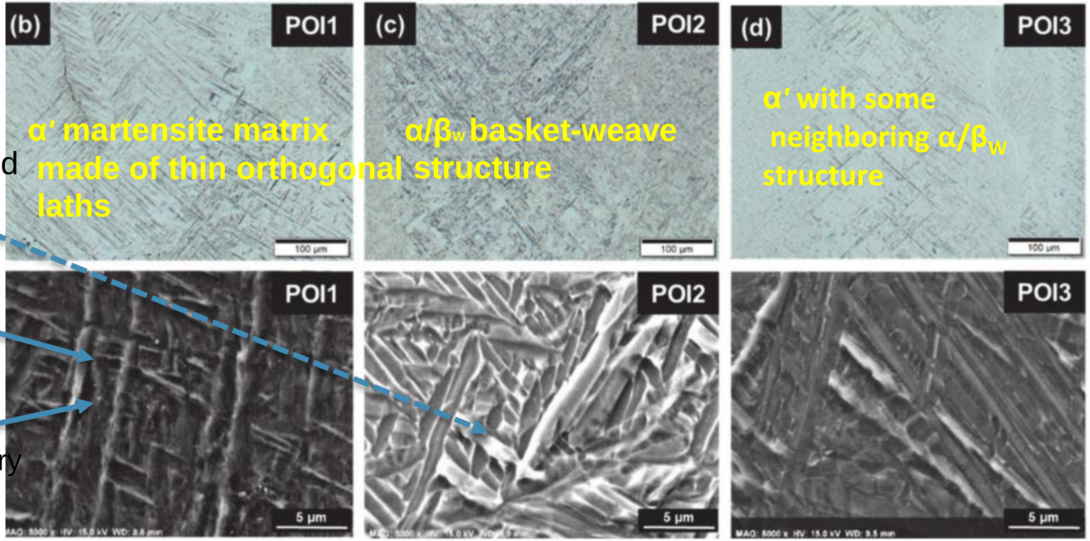




coarsened discontinuous laths of decomposed α’

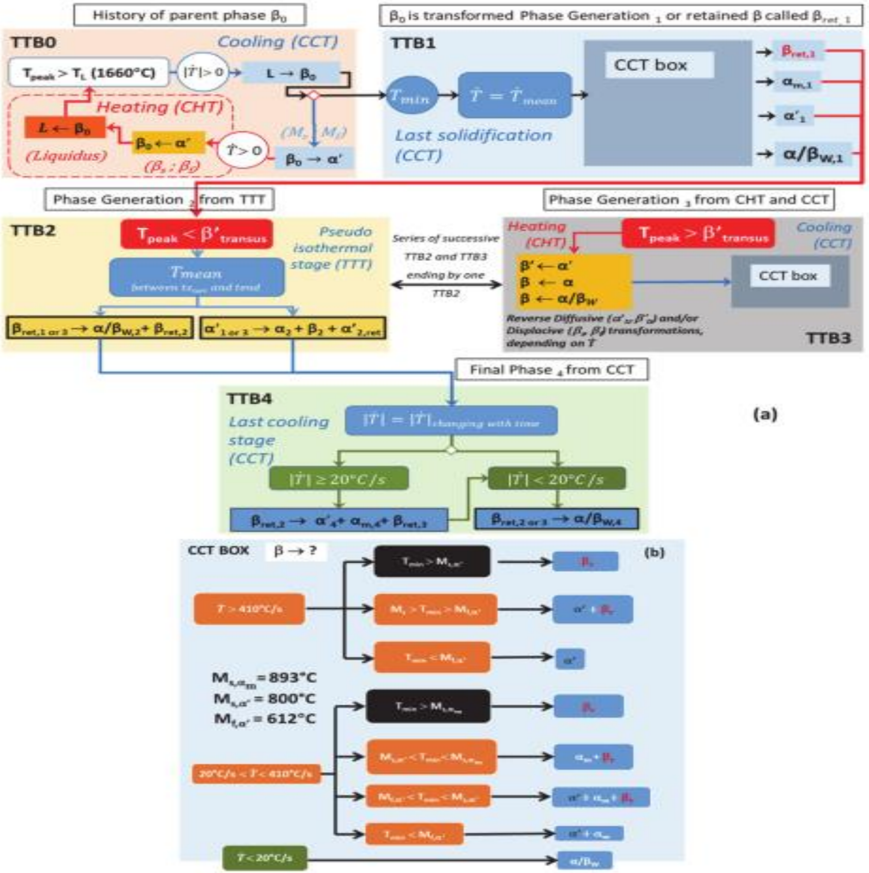
α_m

B prior grain boundary



Tchuindjang JT, Paydas H, Tran HS, Carrus R, Duchêne L, Mertens A, Habraken AM. A New Concept for Modeling Phase Transformations in Ti6Al4V Alloy Manufactured by Directed Energy Deposition. Materials (Basel). 2021

TTB segmentation



Tchuindjang JT, Paydas H, Tran HS, Carrus R, Duchêne L, Mertens A, Habraken AM. A New Concept for Modeling Phase Transformations in Ti6Al4V Alloy Manufactured by Directed Energy Deposition. Materials (Basel). 2021

TTB segmentation

Advantages :

- Robust correlation between Thermal histories and phase genesis

- Identification of optimum microstructures.

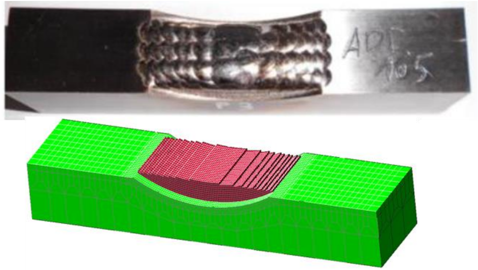
- Taking into account the cooling and the heating effects of the microstructure

- Better explanations of the shift in the critical temperatures

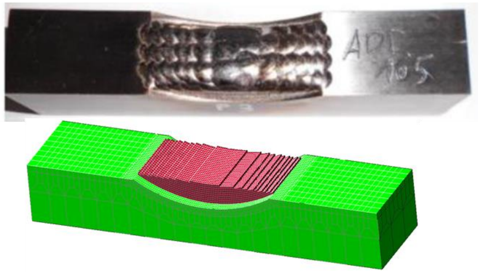
need for automatization of the segmentation procedure to deal with the most highly diverse cases

→ Feed Machine Leaning

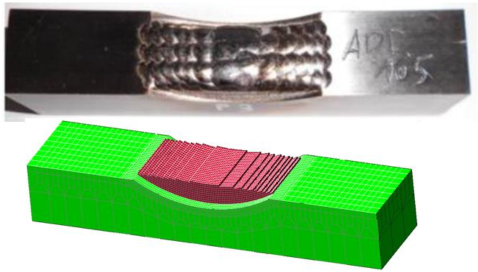
Contents



Contents

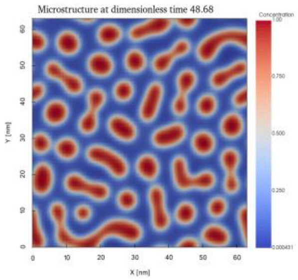


Contents

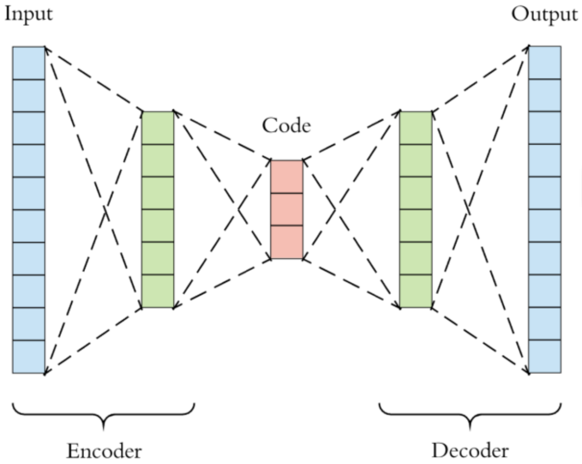


Machine Learning : dimensionality reduction

Initial RGB image



Dimensionality reduction



Further processing

Fetni et al. 2022 – non published results

Machine Learning : dimensionality reduction

Auto-encoders from a numerical point of vue

Original dimension

Latent space

$$\phi : \chi \rightarrow \mathcal{F} \longrightarrow h = \sigma(\mathbf{W}\mathbf{x} + \mathbf{b})$$

$$\psi : \mathcal{F} \rightarrow \chi \longrightarrow x' = \sigma(\mathbf{W}'\mathbf{h} + \mathbf{b}')$$

$$\phi, \psi = \underset{\phi,\psi}{\operatorname{argmin}} \ \|X - (\psi \circ \phi)\|^2$$

$$\mathcal{L}(\mathbf{x}, \mathbf{x}') = \|\mathbf{x} - \mathbf{x}'\|^2 = \|\mathbf{x} - \sigma'(\mathbf{W}'(\sigma(\mathbf{W}\mathbf{x} + \mathbf{b})) + \mathbf{b}')\|^2$$

loss function

Fetni et al. 2022 – non published results

Applications on TA6V

Objectives :

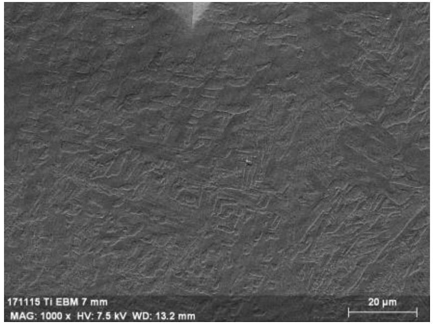
❖ **Dimensionality reduction** of microstructural images of TiAl6V

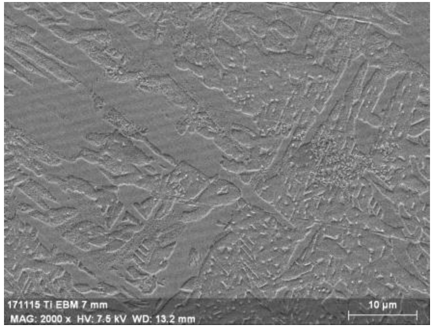
❖ Use the reduced Dataset to make **classification of TiAl6V im**ages into different phases
➔ identify the different phases : α, β, α_m …

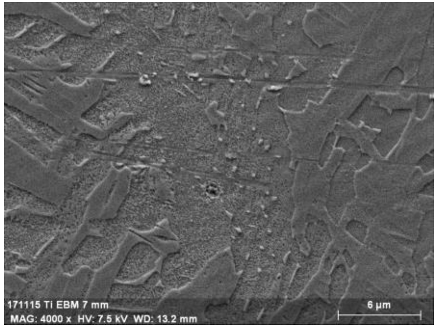
❖ Advanced ML application on TA6V ➔ **phase prediction** basing on the applied thermal histories

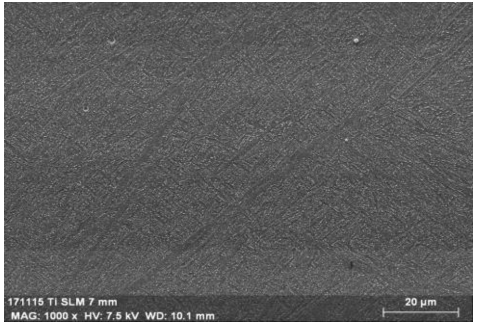
Machine Learning : dimensionality reduction

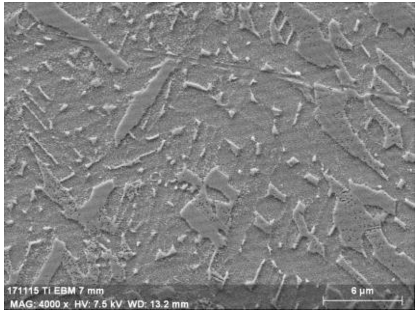
Applications on TA6V ➔ Rich SEM/LOM Dataset

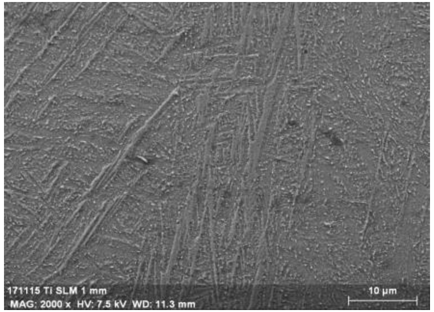


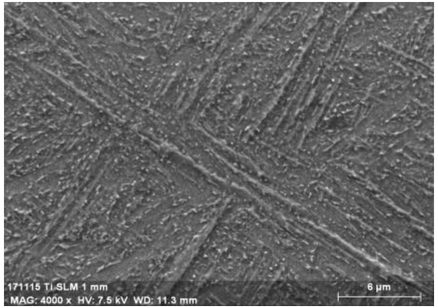


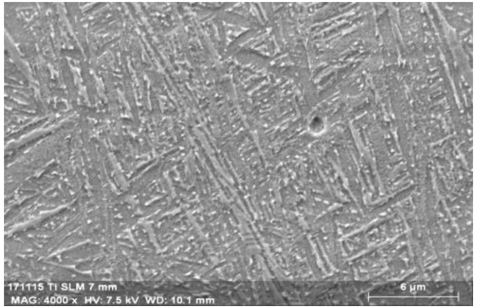








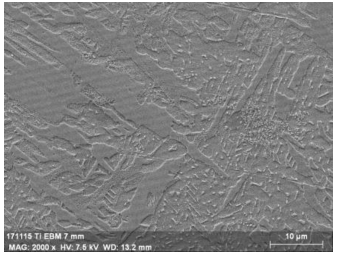




More than 200 SEM images are until now collected: different thermal histories, heat treatments conditions

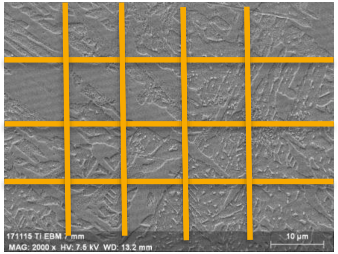
Machine Learning : dimensionality reduction

Applications on TA6V ➔ Rich SEM/LOM Dataset



Slicing into

small parts



Micro still representative

1000 x 750 x3

187 x 250 x 3

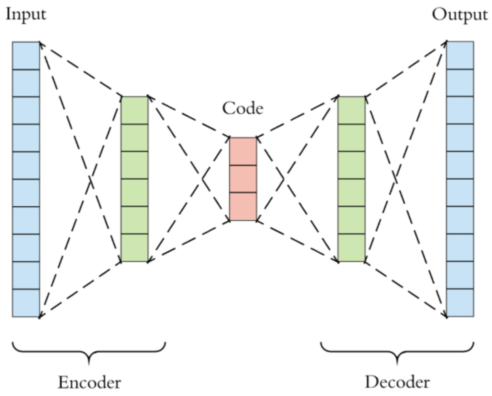
➔One could make classification under an enough rich dataset

➔ Need to build a representative Dataset ; avoid bias

➔ Unstructured data : different scales

Machine Learning : dimensionality reduction

Applications on TA6V ➔ Rich SEM/LOM Dataset



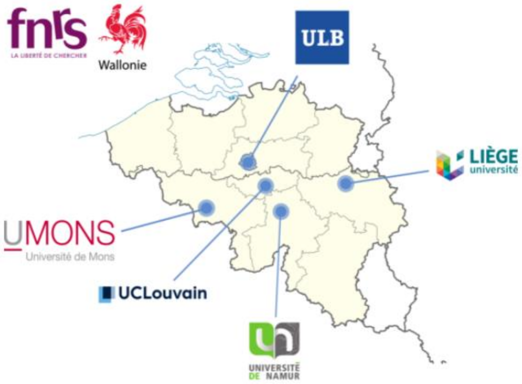
Input image		Code size
187 x 250 x3	→	*2000*

```
Model: "model"
_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
input_3 (InputLayer)         [(None, 187, 250, 3)]     0
_________________________________________________________________
sequential (Sequential)      (None, 2000)              280502000
_________________________________________________________________
sequential_1 (Sequential)    (None, 187, 250, 3)       280640250
=================================================================
Total params: 561,142,250
Trainable params: 561,142,250
Non-trainable params: 0
```

Reduction ratio: 1/70

Applications on TA6V ➔ computing resources

CÉCI

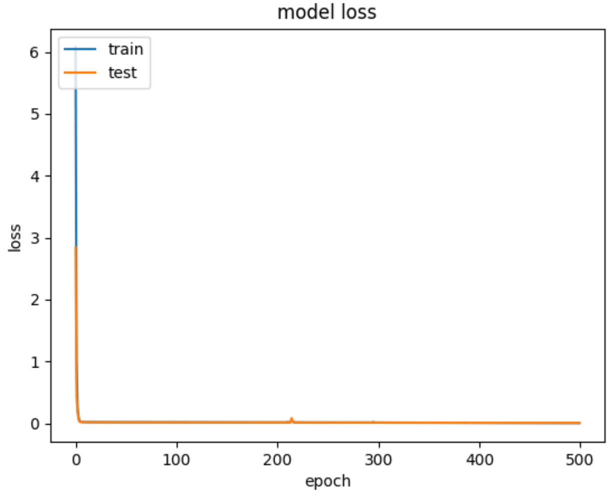


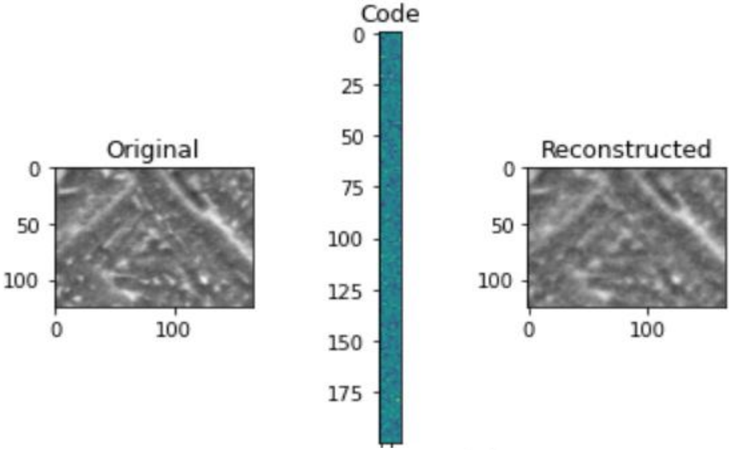
HPC Computing

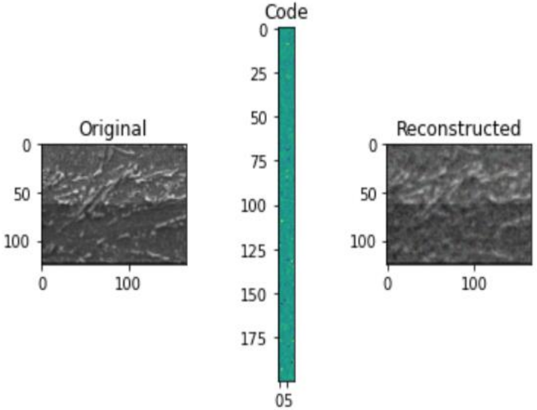
Hercules2	UNamur	Naples 2 GHz SandyBridge 2.20 GHz	1024 (30 x 32 + 2 x 64) 512 (32 x 16)	64 GB..2 TB	10 GbE	NFS 20 TB	None	15 days	serial / SMP

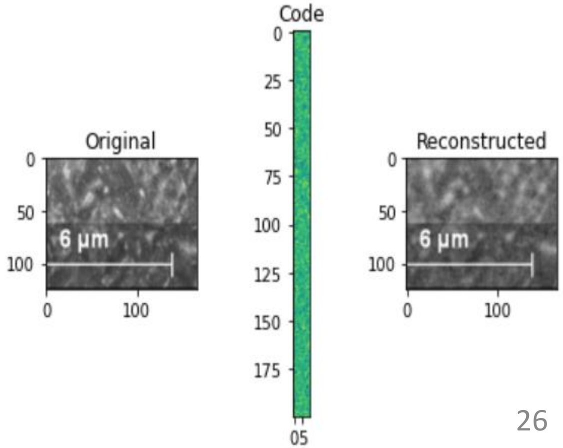
Machine Learning : dimensionality reduction

Applications on TA6V ➔ Rich SEM/LOM Dataset





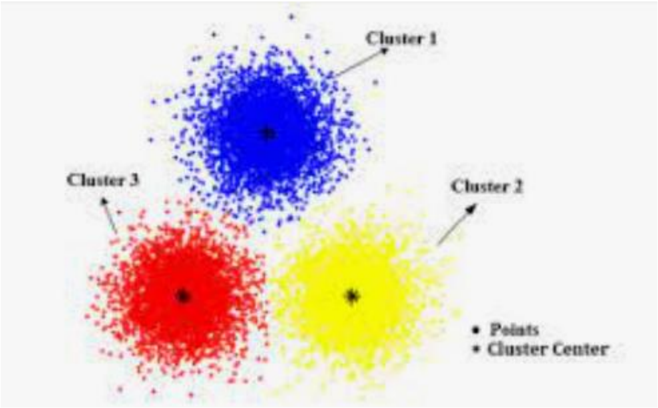




Hyperparameters of the auto-encoder model : 1 hidden layer, ‘adamax’ optimizer

Training CPU time: 20:30:27 ; batch_size=264 ; maximum memory needed: ≈ 83GB

K-means Clustering



- *Unsupervised learning*
- *Apply on the reduced dataset χ*

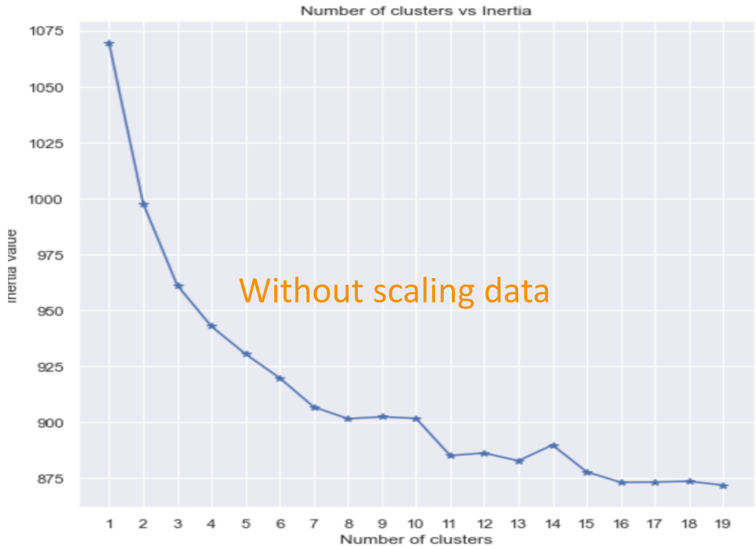
(latent space :2000)

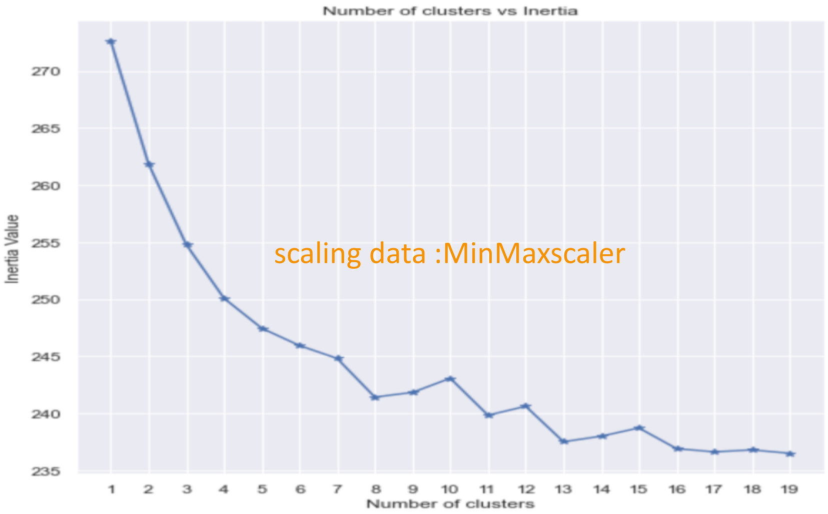
- *Investigate the capabilities of Machine Learning*

To deal with the complexity of TA6V microstructures and identify the different phases.

Machine Learning : Classification - Clustering

K-Means Clustering





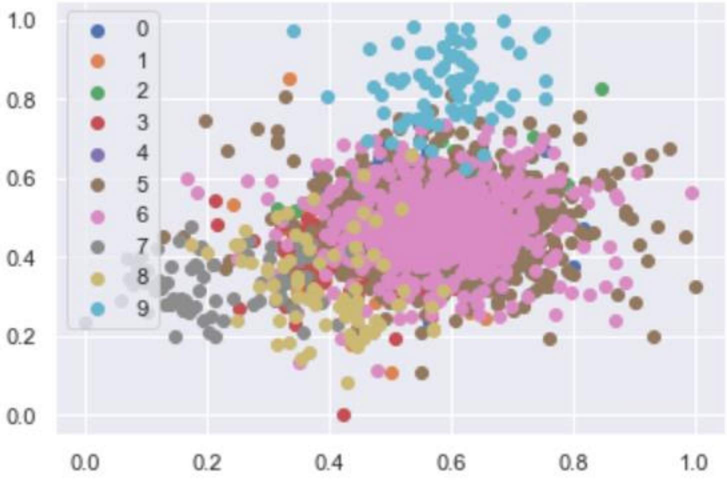

```
kmc.labels_
✓ 0.4s

array([2, 1, 2, ..., 9, 9, 8])
```

- ❖ For 20 clusters, the inertia still high.
- ❖ Data scaling enhances the improvement of the inertia value.
- ❖ However, kmc could place each sample in the associated class.
- ➔ The microstructural-images based dataset could clustered into 19 groups for instant.
  ➔ more data processing should be applied (better choice of representative micros, deal with bias ..)

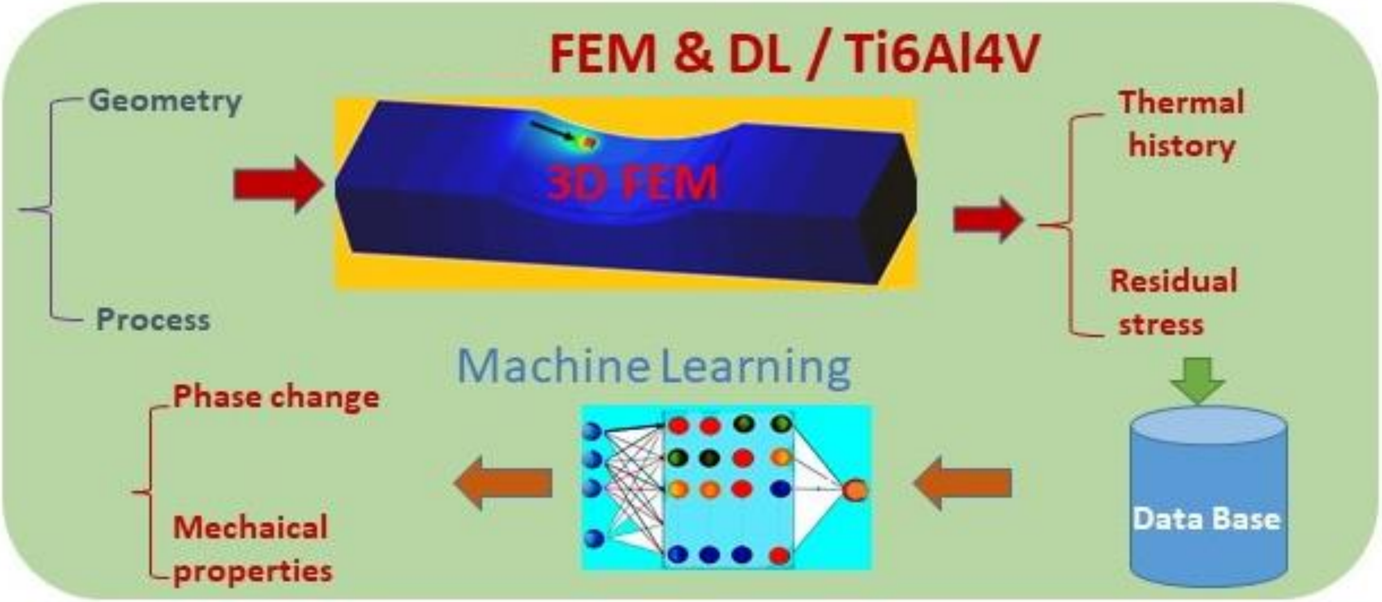
Machine Learning : Classification - Clustering

K-Means Clustering

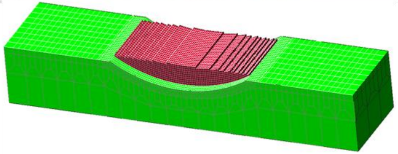


- Clustering results for 10 clusters (for simplification purposes).
- First appearance of some distinguishing groups
- Note that the size features (2000) is relatively high for a good clustering ➔ need to decrease to (200 -350)

Machine Learning : Proposed Framework



Contents



Conclusions

❖ Investigations of TiAl6V using : Finite Element Modeling, Microstructural investigations and Machine Learning.

❖ Finite Element Modeling ➔ prediction of the Thermal history in all parts of the Clad.

❖ TTB allow Robust correlation between Thermal histories and phase genesis.

❖ Implementation of Auto-Encoders as practical Machine Learning technique for the compression of microstructural images.

❖ Further work : Feed ML algorithms (auto-encoders, k-means clustering, decision tree, reinforcement learning techniques …) with two types of datasets: FEM-based and from experiments (SEM, LOM, micro-hardness maps ..) ➔ Control the phase-changes and mechanical properties in TiAl6V ➔ improve materials design.

Thank you very much for your attention