The recourse to artificial intelligence to design Co-free wear-resistant alloys

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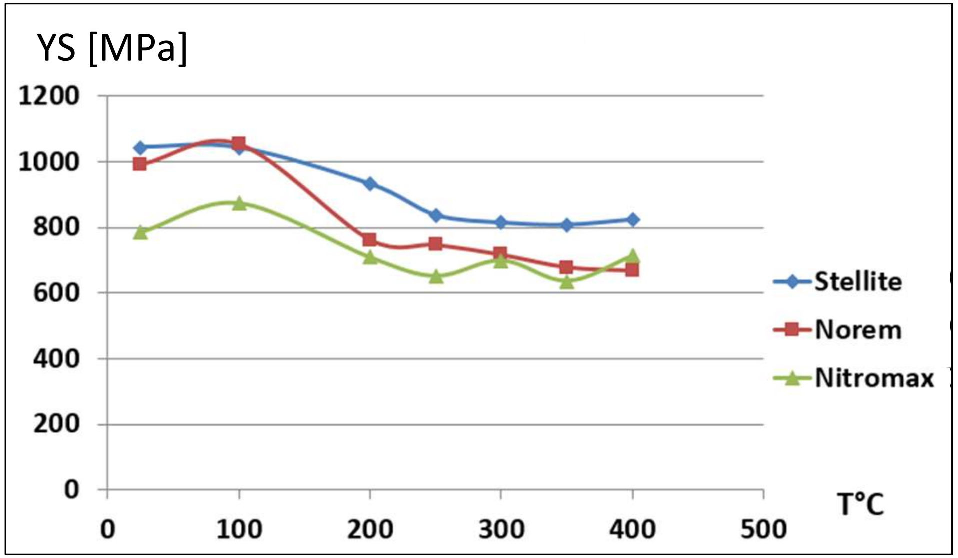
Context

- Stellite alloys (Co-Cr) : currently used in nuclear industry as welded wear-resistant coating
  - Issue : Co presence (mainly irradiation)

- Several alloys developed for Stellite replacement
  - NOREM and Nitromaxx : Fe-Cr-Si-C-**N** [1]
  - FeCrB : Fe-Cr-Si-C-**B** [2]
  - Issue : lack of high temperature (>180°C) mechanical properties stability



%wt.	Fe	Cr	Si	Mn	Mo	Ni	C	B	N
NOREM	Bal.	25	3	4	2	4	1.3	-	0.2
FeCrB	Bal.	20	1	-	-	-	1.8	0.7	-

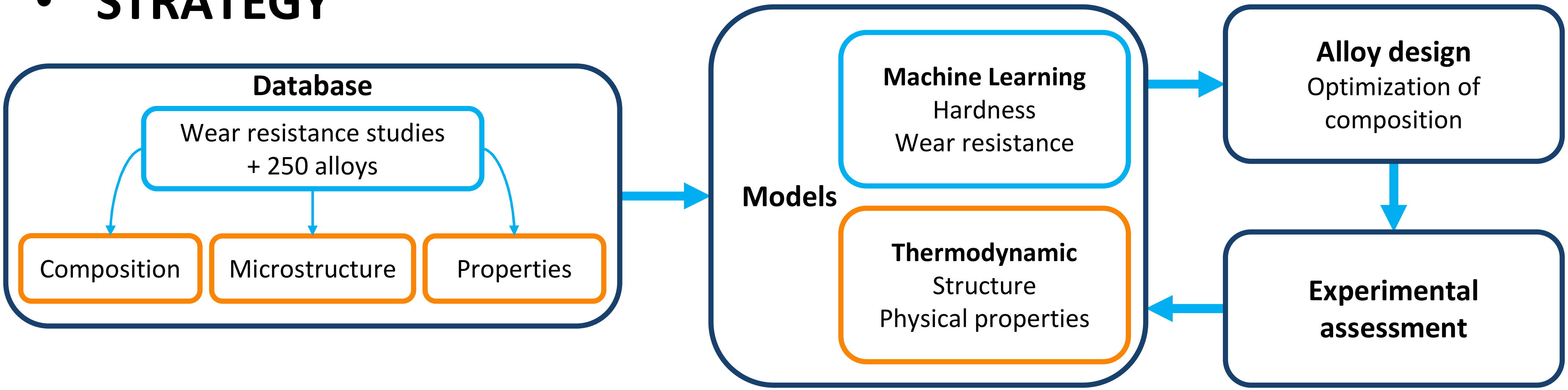
[1] EPRI Patents, **1989**
[2] Yoo et al. , *Journal of Nuclear Materials*, **2006**

Purpose et strategy

- **PURPOSE**

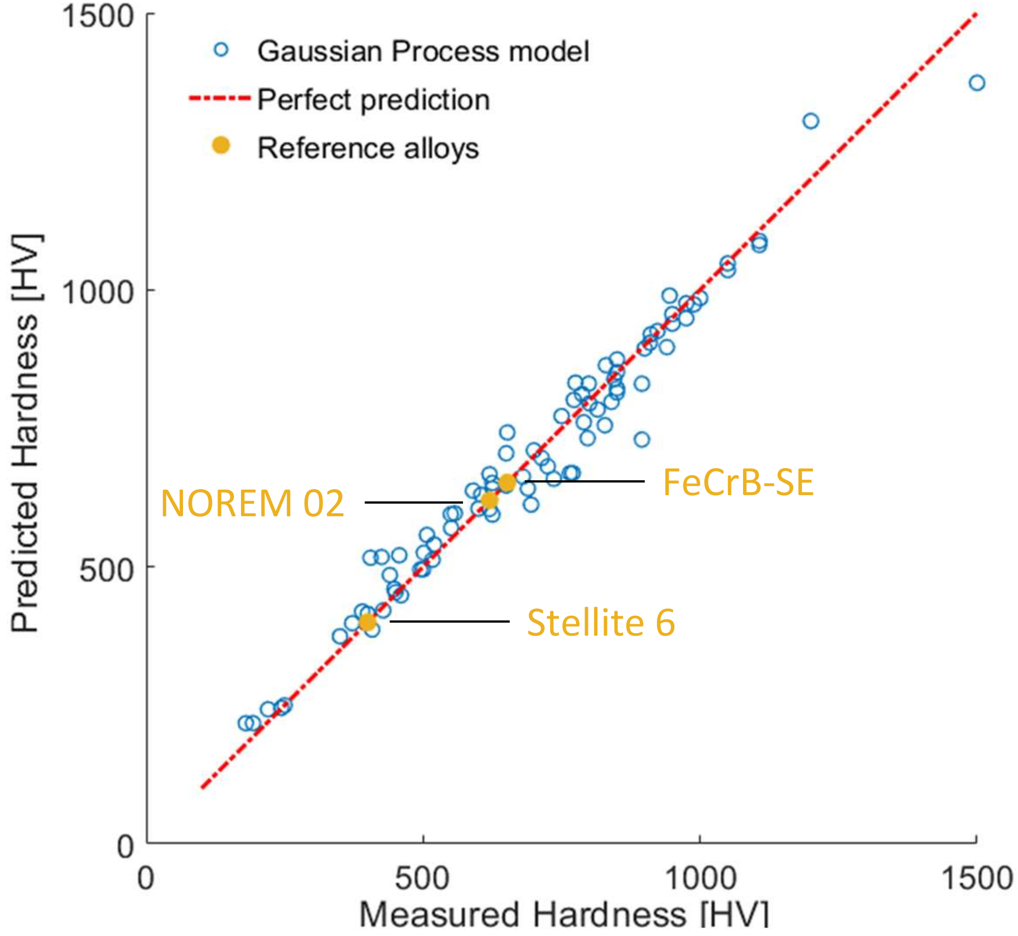
  Design of improved alloys :
  - Co-free and Fe-rich alloys
  - Mechanical and tribological properties similar to Stellite

- **STRATEGY**



Machine learning models
Hardness

- Correlate hardness and alloy composition
  Using ML [3], multi-variable regression
  → Creation of the model
  Learning from bibliographic data
  → Confirmation of the model
  Prediction of hardness for bibliographic alloys
  With only Fe-based alloys



> ➢ Satisfactory agreement between experimental data and predictions
> *Stellite used only as reference*

[3] C. E. Rasmussen, C. K. I. Williams, *Gaussian Processes for Machine Learning*, **2006**

Machine learning models
Wear resistance (1)

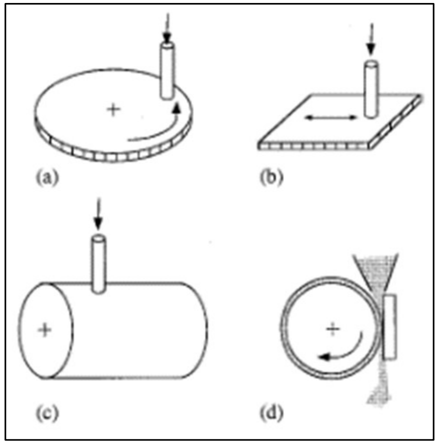
- Issue : scarce experimental data difficult to use for ML

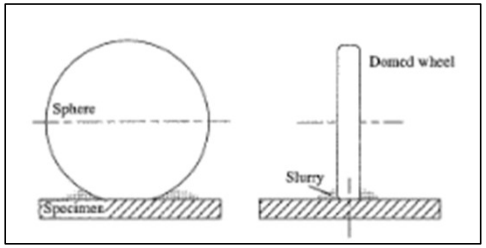
- Different experimental conditions

Configuration of test [4]
Shape of the counterpart [4]
Load
Temperature
Environment

- Measured data

Depth, volume of wear track
Wear rate
Friction coefficient





[4] B. Bhushan, *Modern Tribology Handbook*, **2000**

- But, often a paper compares different alloys using the same set of conditions

- Ranking alloys :
  Pair-wise comparison algorithm :
  SpringRank
  Ranking by performance

Machine learning models
Wear resistance (2)

- Comparisons matrix built from wear tests results :
  - 35 compared alloys
- 3 types of comparisons matrix :
  - « With weight» : from raw data (wear tests results)
  - « Without weight » : if $\frac{v_3}{v_2} \neq 0$, replaced by 1
  - « Smooth weight » : *log(Weight)+1*
- SpringRank algorithm :
  - Search a minimum energy with consecutive permutations

> ➢ Same SpringRank scores as a function of matrix
> ➢ « With weight » matrix chosen for next step
> ➢ Rank 1 attributed to the better SpringRank score
> *Alloys ranked from 1 to 35*

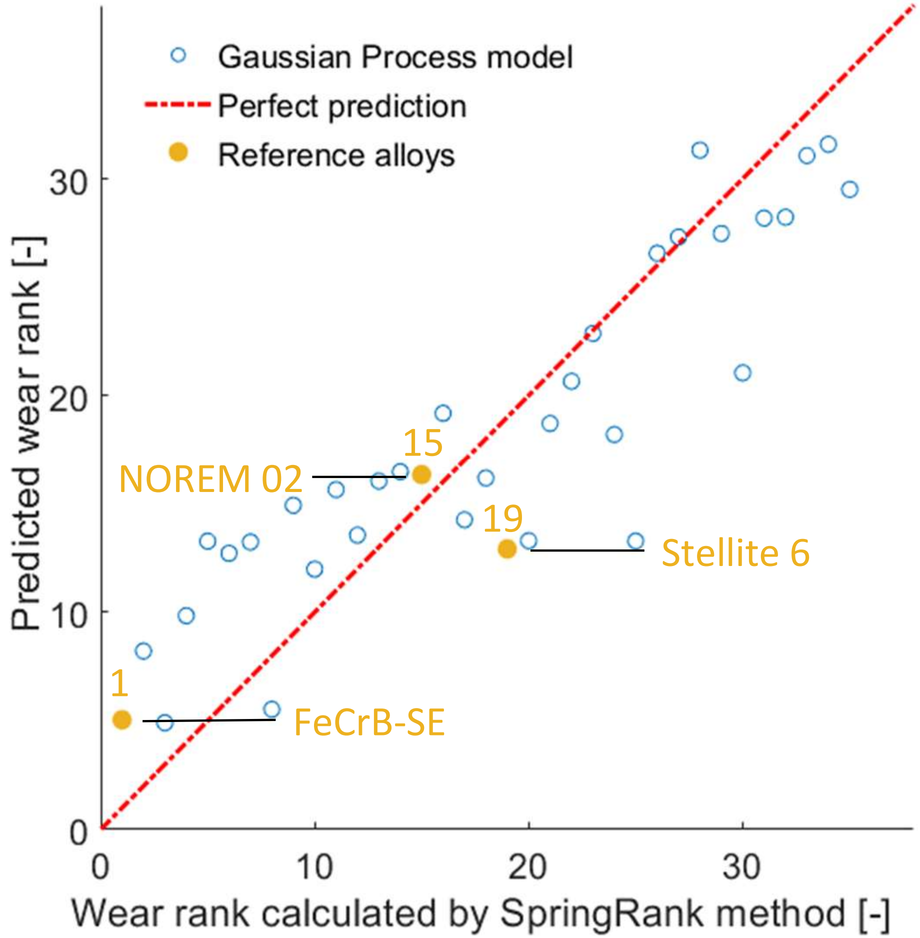
	A_1	A_2	A_3	A_n
A_1	0			
A_2		0	0	
A_3		v_3/v_2	0	
				0
A_n				

Comparisons matrix in case of A_3 is better than A_2, with raw data

Machine learning models
Wear resistance (3)

- Correlation wear rank and composition
  Using ML, same method as hardness

- Model using Fe-, Ni- and Co-based alloys

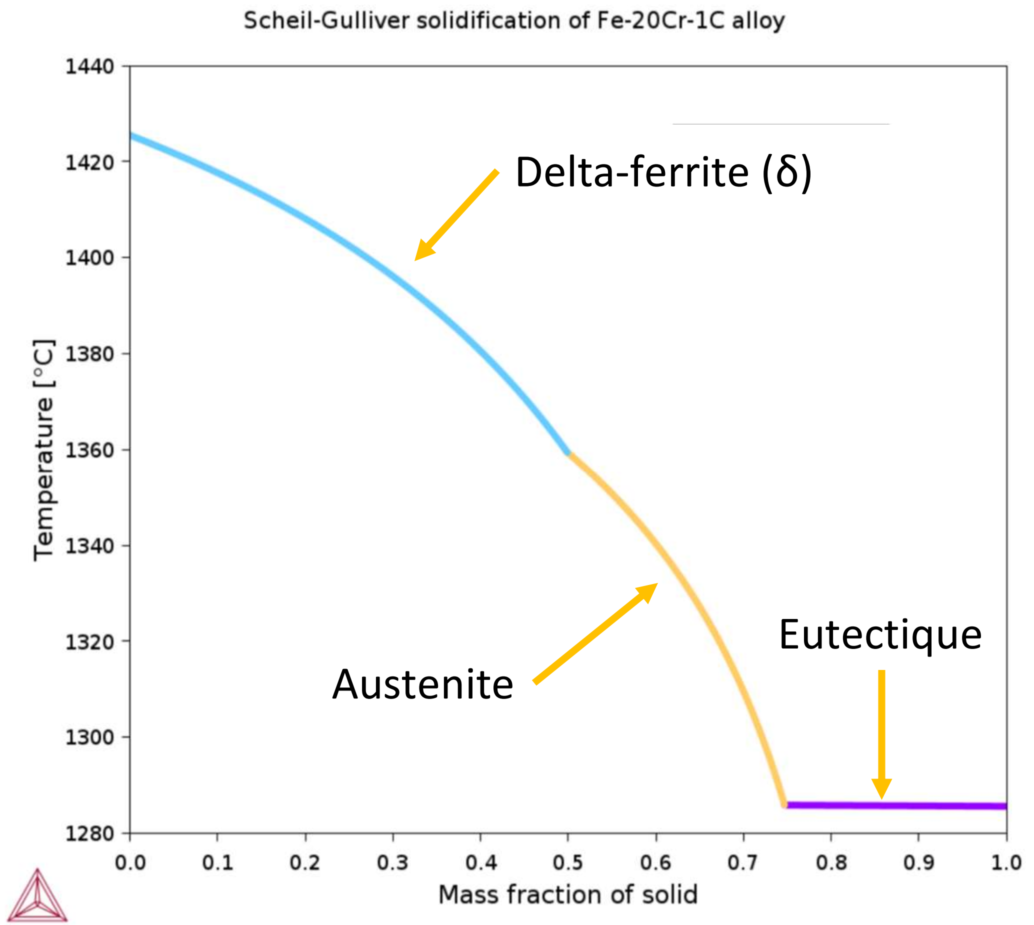


> ➢ Satisfactory agreement between experimental data and predictions
> ➢ Predictions are possible from any composition

Thermodynamic models

- CalPHaD : Calculation of PHase Diagrams
  Thermo-Calc ® software, TCFE9 database
- Scheil-Gulliver model of solidification

Criteria :
- Identified structure
  - Delta-ferrite (δ, hot cracking resistance)
  - Austenite
  - Eutectic(s) mixtures : (carbides/borides) + austenite
- Corrosion resistance
  - Cr content > 16%wt. in austenite



Alloy design

- Searching for an original optimized chemical composition using a multi-objectives genetic algorithm [5]
  - Objectives : To minimize or maximize
  - Constraints : To select alloys according to specifications

- More than 1000 « non-dominated » compositions
  - 2 alloys selected for experimental assessments (AS1 and AS2)

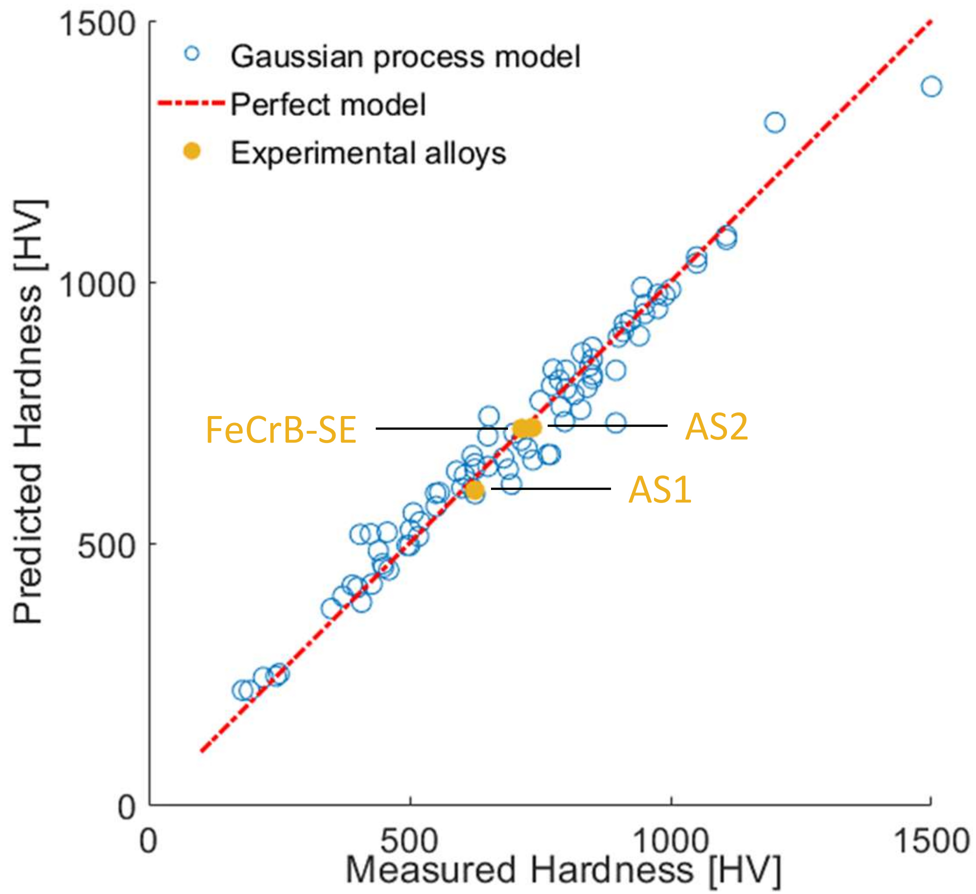
%wt.	Fe	Cr	Si	Mn	Mo	Ni	Nb	C	B
AS-Series	Bal.	15-30	<1.5	<5	<5	<5	<3	<2	<2

- Ingots elaboration
  - Cold crucible induction melting
  - At MINES Saint-Etienne

[5] E. Menou, *Modelling Simul. Mater. Sci. Eng.*, **2016**

Experimental assessment

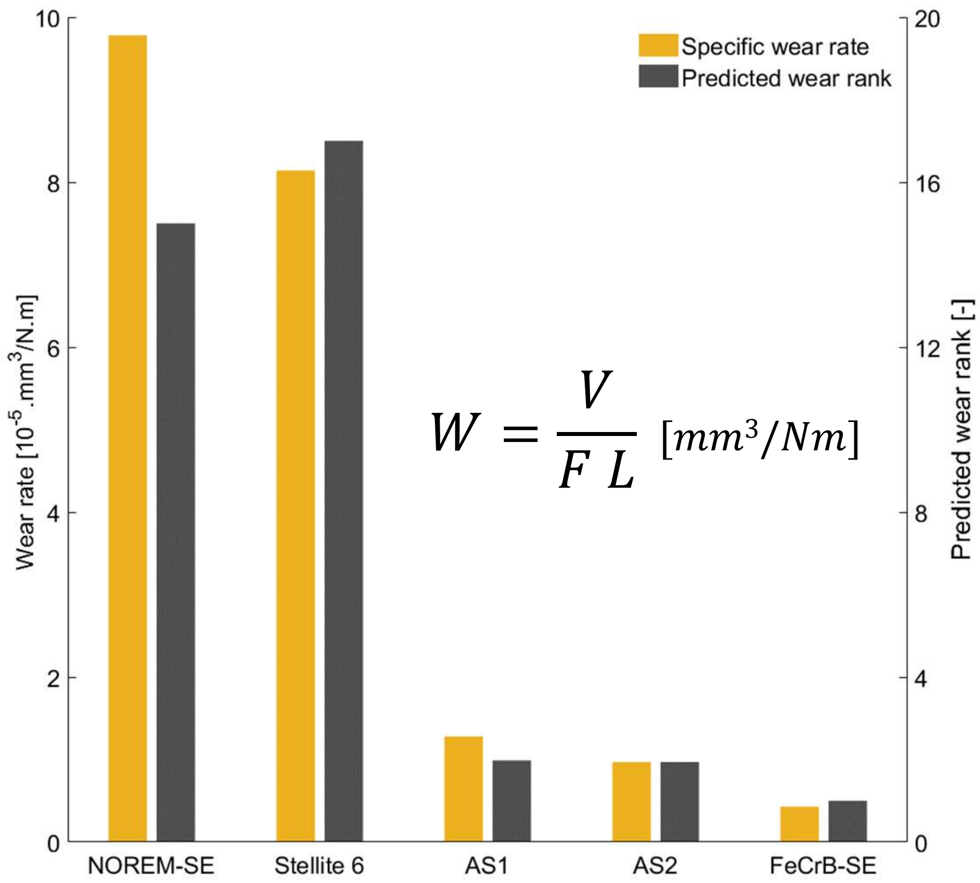
- Experimental assessment
  - **Vickers hardness**



Experimental assessment

- Experimental assessment
  - Vickers hardness
  - Microstructure et comparison with predictions
  - **Wear tests**

- Experimental conditions
  Ball-on-disc
  - Normal load 10N
  - Room temperature
  - Without lubricant
  - Tungsten carbide (WC) ball



Conclusion

- Different tools of machine learning et thermodynamic have been used for the design of new wear-resistant alloys to replace Stellite grade :
  - Hardness : multi-variable regression
  - Wear resistance: coupling pair-wise comparison ranking and multi-variable regression
  - Thermodynamic : Calphad method with Scheil-Gulliver model of solidification
  - Alloy design : multi-objectives genetic algorithm

- 2 original and optimised alloys have been elaborated (AS1 and AS2) and tested :
  - Confirming hardness and wear resistance models
  - Ang giving promising results