Amaya Igartua, Borja Coto, Iban Quintana, Cristina Monteserin, Jon Lambarri, Borja Zabala, Iker Esnaola,TEKNIKER

Modeling Activities to optimize materials properties, processes and performance. Ontologies, Dissemination

Tekniker | EIBAR | 24/02/2021

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Content

Materials and Product Optimization:

- Atomistic modelling and molecular dynamics **nanocomposites and nanopigments**,
- *Borja Coto (borja.coto@tekniker.es ; Doctoral Thesis)*
- Optimization of a **nebullizer** design, *Jon Lambarri (jon.Lambarri@tekniker.es)*

Process Optimization:

- Numerical modelling in **Laser** processing, *Jon Lambarri*
- **Cutting** operations, *Itxaso Cascón (Itxaso.gascon@tekniker.es)*
- **Curing** treatment, *Cristina Monteserin (cristina.monteserin@tekniker.es, Doctoral Thesis)*

Performance Optimization:

- Modelling **elastomers and Bearings** (Aitor Fernandez, aitor.fernandez@tekniker.es)
- **Moulds durability** in function of the type of failure modes, *Borja Zabala*
- *(Borja.zabala@tekniker.es; Doctoral Thesis)*

Ontology

- OntoCommons Project, Iker Esnaola, iker.Esnaola@tekniker.es

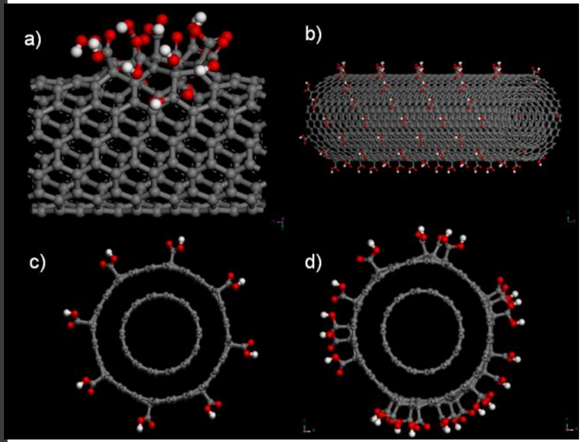
Dissemination

- EMMC 2021, 2-4 March

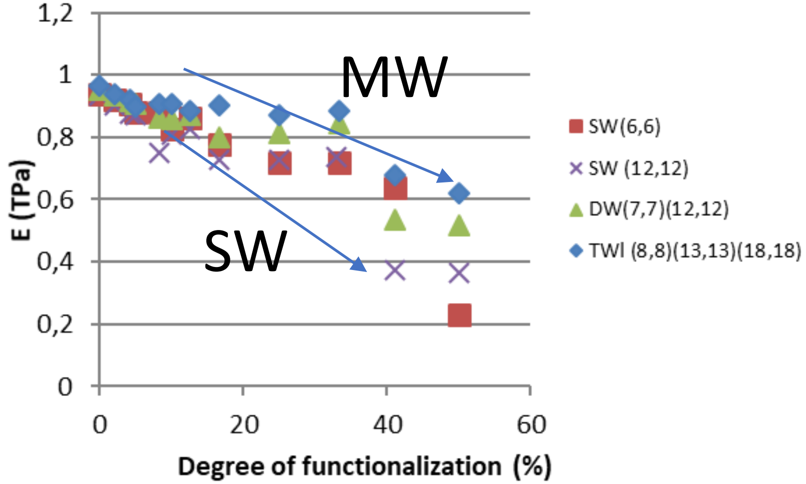
Materials Optimization: Polymer Composites Functionalization

Objective: innovative polymer composites filled with CNT to obtain **nanostructured materials**

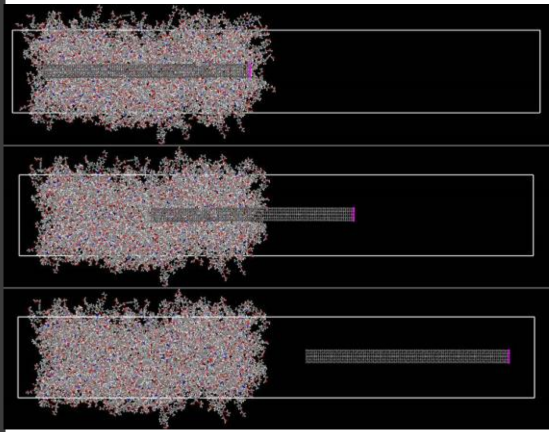
Modelling goal: Study the influence of **functionalization on mechanical properties** of CNTs. **Modelling tool: MD** (Acceleris, Materials Studio)

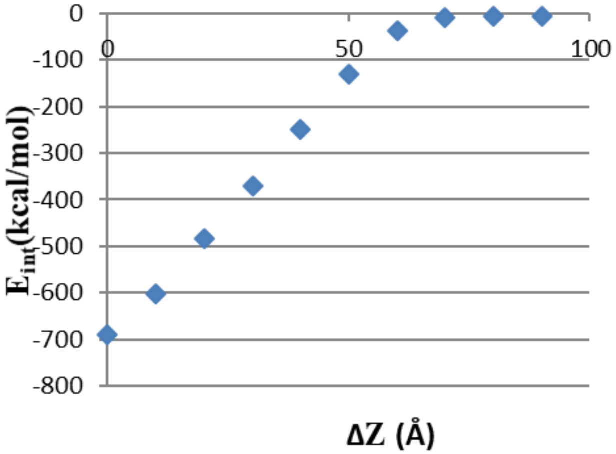


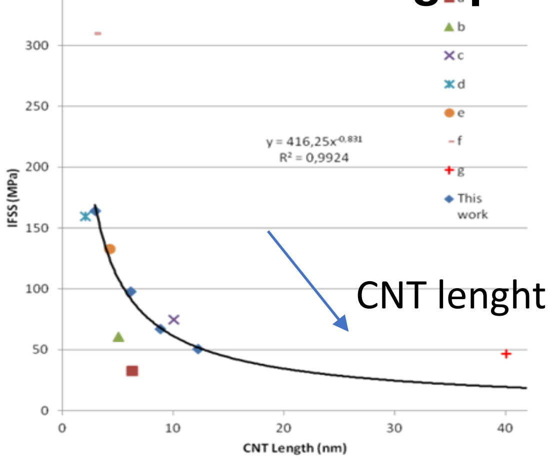
- Young's modulus **decreases** as **% of functionalization increases**.
- **The decrease** is **less critical in MWCNT** than in SWCNTs



- **MD modelling:** Interphase Interaction between CNT & polymeric matrix **simulating pulling out** of the CNT.







Interfacial Shear Strength vs Length of CNT.

B. Coto et al. Computational Materials Science. Vol 50, 12, 2011, pp 3417–3424

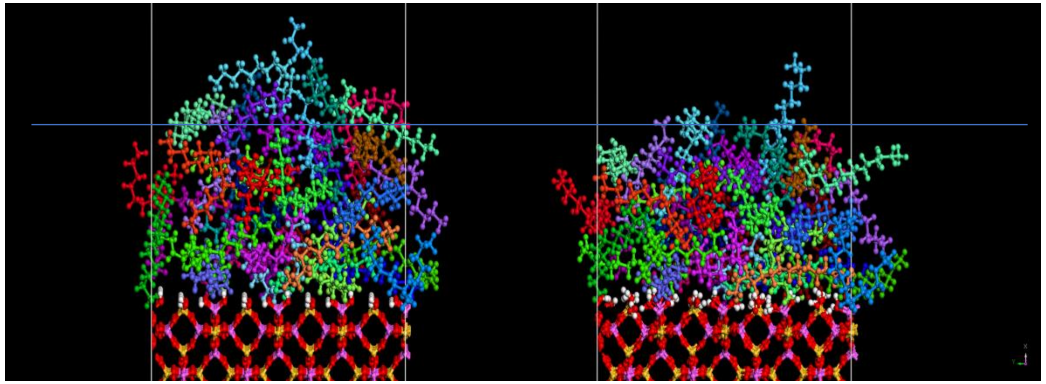
EU project

Materials Optimization: Absorption PCMs/Pigments

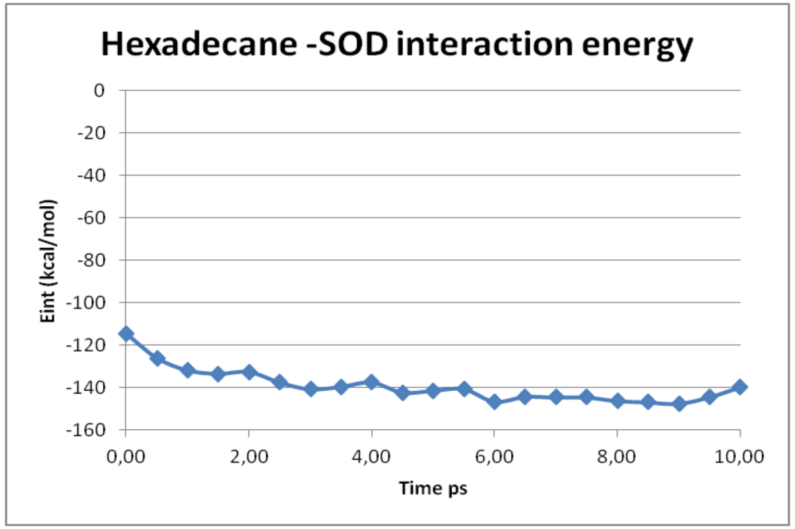
NANO PIGMY EU project

Project Objective: develop multi-functional and cost-efficient **ceramic nanopigments** for paint, plastic and concrete

- **Modelling Tools: Atomistic Monte Carlo simulations to study** absorption of molecules (PCM) in porous medium



Configurations of hexadecane molecules adsorbed on a surface before and after 10 ps of MD run



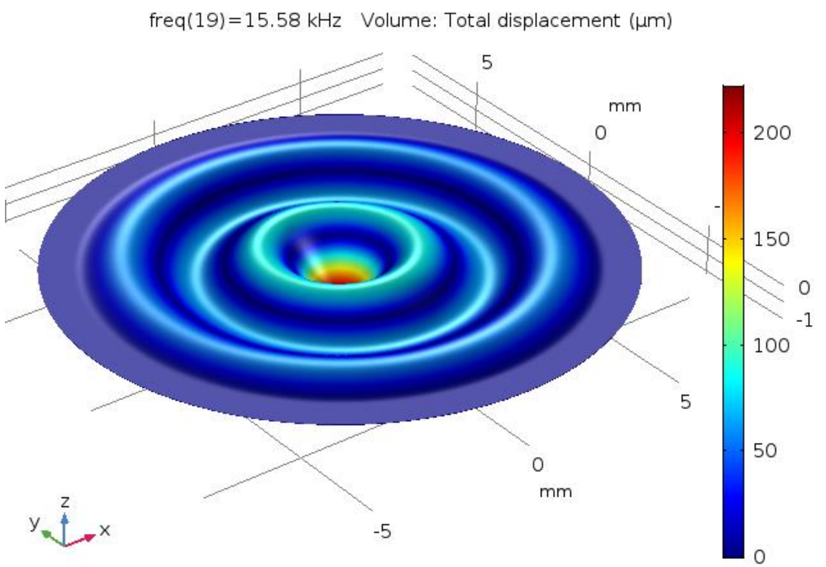
Evolution of the interaction energy between hexadecane molecules layer and the SOD surface

- Evolution (10ps) of **adsorbed molecules** to determine their suitability to be adsorbed in a nano porous surface
- The MD simulation **show the stability** in time of the absorbed layer

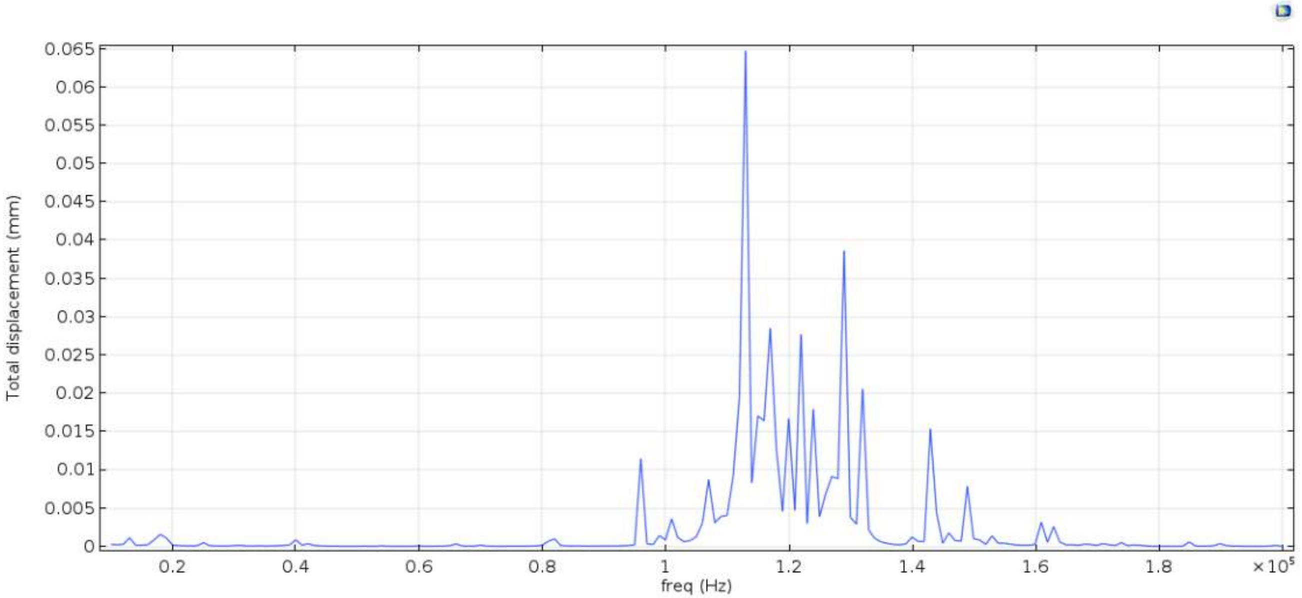
The Nanopigmy project has received funding from the European Community's Seventh Framework Programme (FP7-NMP-2011-SME-5) under grant agreement no 280393.

Product Optimization: Optimization of a nebulizer design

- **Objective**: Optimize a nebulizer design and find appropiate operation parameters
- **Modelling Tools:** Multiphysics COMSOL



Piezoelectric simulation of the membrane

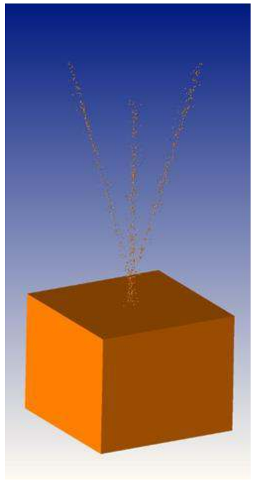


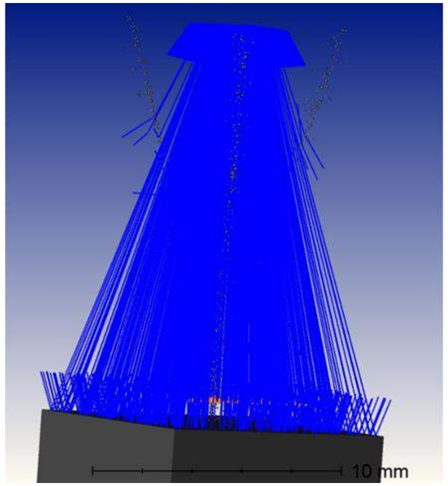
Output : Optimized geometry and frequency spectrum

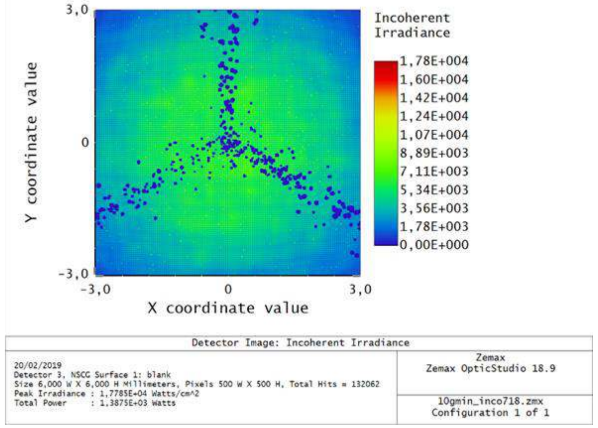
The research leading to these results was carried out in cooperation with **LAINO MEDICAL**

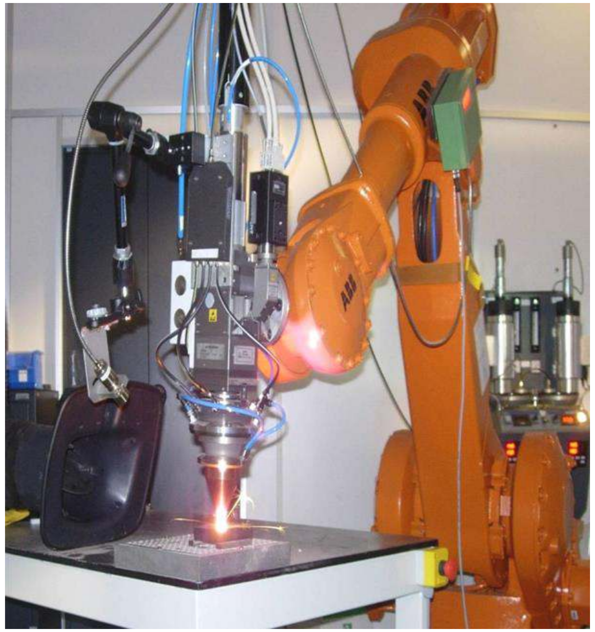
Process Optimization: Ray tracing during Laser Melting Deposition

- ***Goal:*** Study **laser-matter interactions** for laser additive manufacturing of metals to **predict the thermal and mechanical response** of the parts
- ***Modelling Tools:*** *ZEMAX, OpenFOAM, SYSWELD*





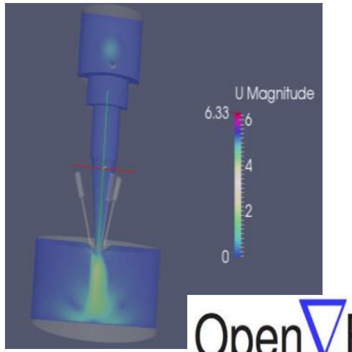




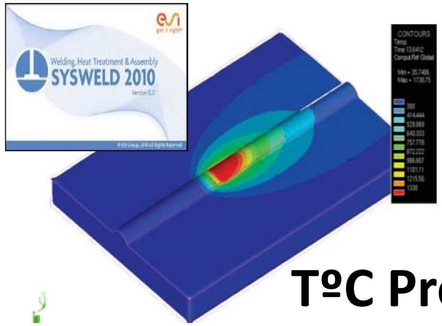
Import **powder cloud**

Ray tracing from a laser source to the substrate

Output : **Effective power density** distribution for thermo-mechanical FEM simulation

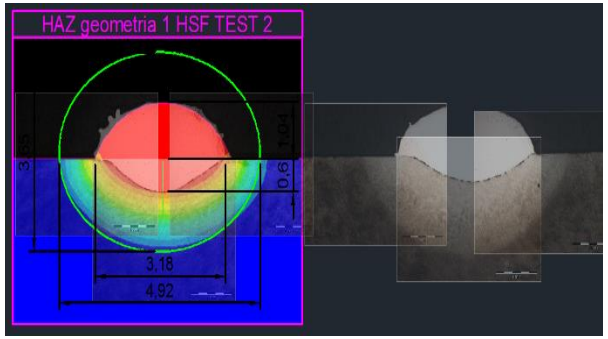


OpenFOAM



(a) External surfaces isotherms

TºC Processing



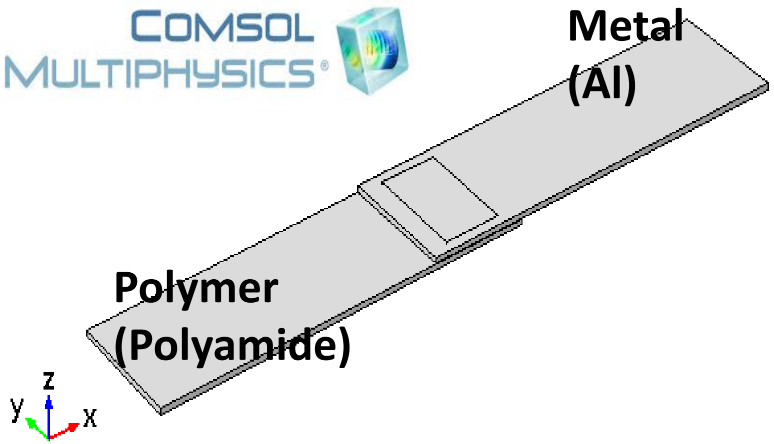
Deposited track geometry

Process Optimization: Laser joining hybrid polymer-metal

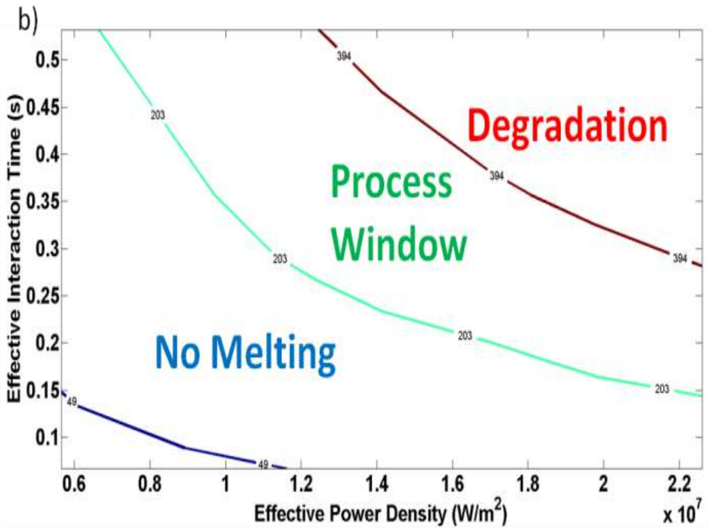
Goals: Obtain the process **parameter window** avoiding lack of melting or polymer degradation

Modelling tools: COMSOL Multiphysics

Applications: Hybrid components for lightweight structures



Test part configuration



Numerical parameter map

Funds from the European Union's Seventh Framework Programme (FP7/2007-2013) under grant agreement 309993. PM Join. **Partners:** Fraunhofer ILT, Faurecia, Valeo, PSA, Armines, Andaltec, Lasea, Tekniker

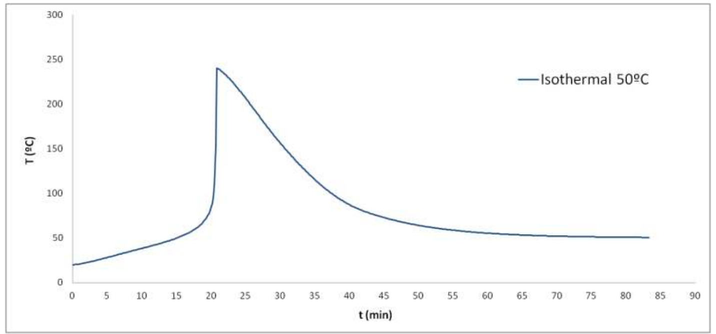
Process Optimization: Curing epoxy resins

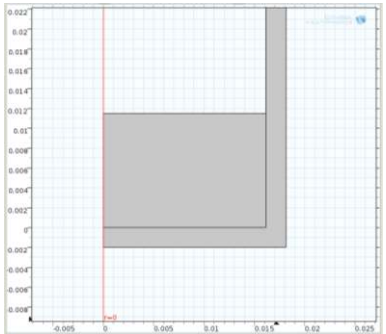
EMACOMP project

Objective: to study the **curing kinetic** of an **epoxy resin** and the relationship between **the curing process parameters** and final **properties** of the thermoset networks

Modelling Tools: FEM Simulations, COMSOL, **Goal**: Coupling between **heat transfer & chemical kinetics**

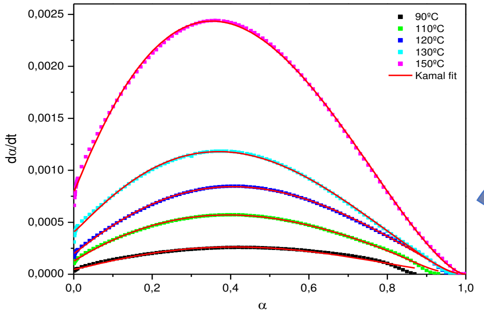
Objective	Impact
Curing **evolution** in a viscoelastic thermoset polymer resin	Increase **process control**
Predict and optimize curing cycles	increase **process efficiency**
Obtain **high degrees** of **curing**	Improve **quality**
Avoid heat degradation	increase **durability**
Reduce curing times	Reduce **cost**





Process Optimization: Curing epoxy resins

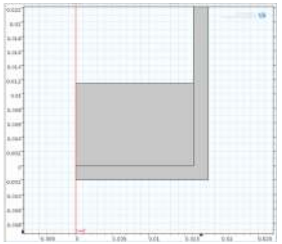
1. **Thermal characterization** of the curing kinetics

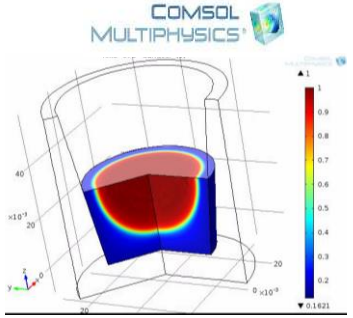


2. Obtaining of a **kinetic model** corresponding to the curing behaviour of a specific system (resin-curing agent)

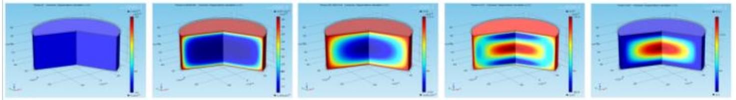
$$d\alpha/dt = (k_1 + k_2\alpha^m)(1-\alpha)^n$$

3. **Simulation of a real piece**, coupling chemical kinetics and heat transfer, using Levenberg-Marquardt **non-linear regression analysis**



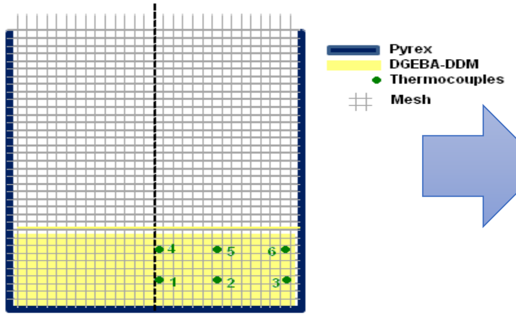


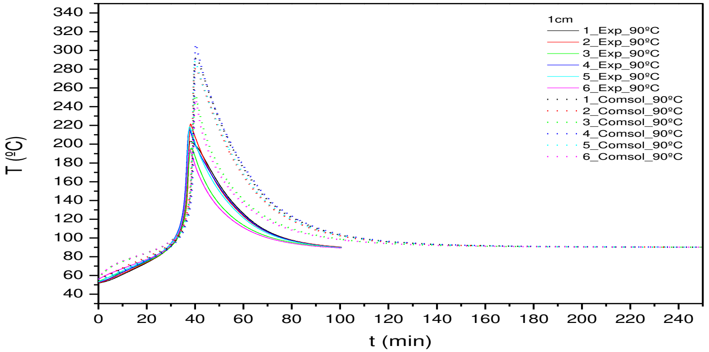
Mapping **TºC and curing degree** at any point and any time



Good correlation in TºC values. Simulation **vs** Experimental

4. **Validation of simulation** (experimental test)



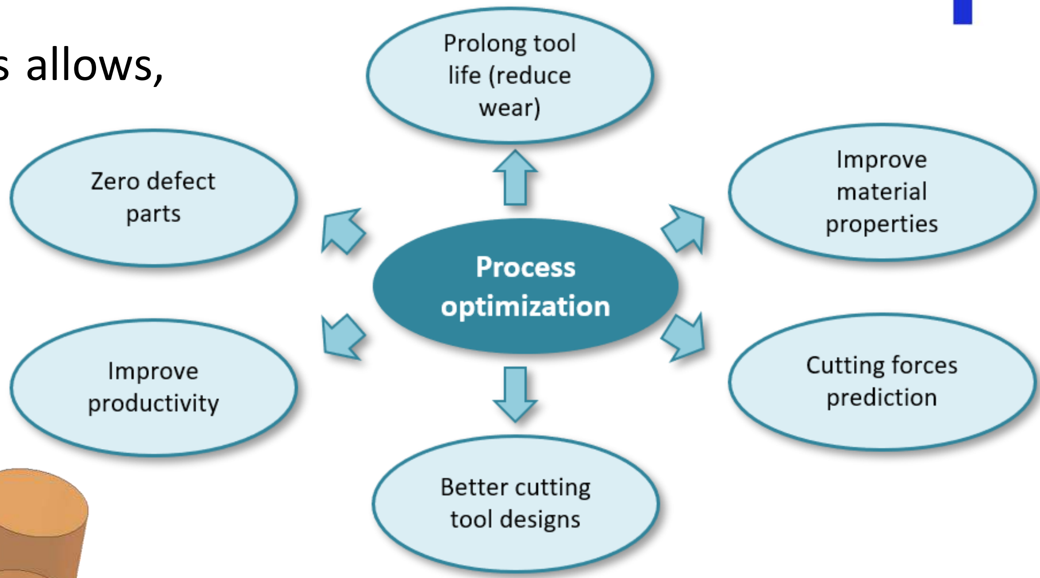


C. Monteserín, M. Blanco, J.M. Laza, E. Aranzabe, J.L. Vilas. "Thickness effect on the generation of temperature and curing degree gradients in epoxy–amine thermoset systems" Journal of Thermal Analysis and Calorimetry (2018) 132:1867–1881

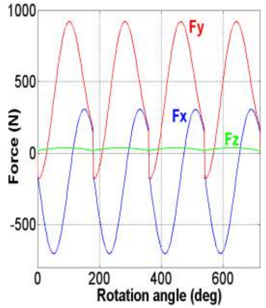
Process Optimization: Cutting and Machining

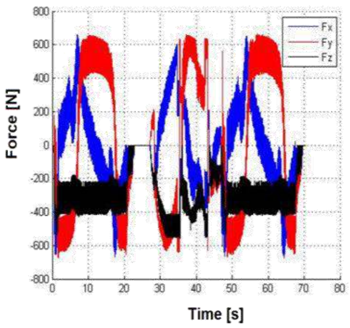
Objective/Impact: optimization of **manufacturing** processes. Models allows,

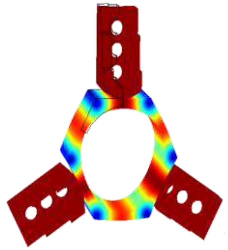
reducing the number of experiments and **reducing costs.**

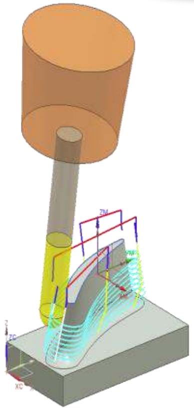


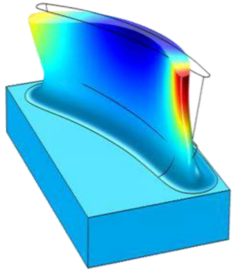
- Cutting and machining (**Prediction of cutting force**
  - stability (chatter and vibrations)
  - Material removal
  - **Surface finishing forecast**
  - CAD/CAM Integration
  - Chip formation (**mechanical & thermal effects)**
  - **Clamping distortion**
- Heat Treatments
- Modal analysis
- Tool design
  - Tool geometry and performance analysis
  - Design of a chip breaker
  - Better milling tooth paths

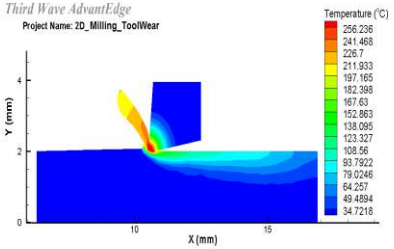




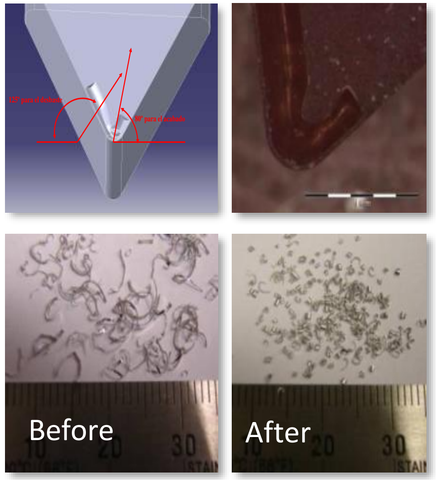








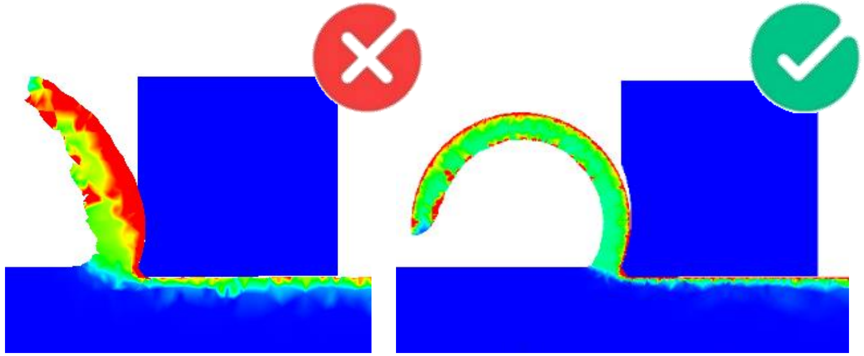
Design of a chip breaker



Process Optimization: Modelling tool design

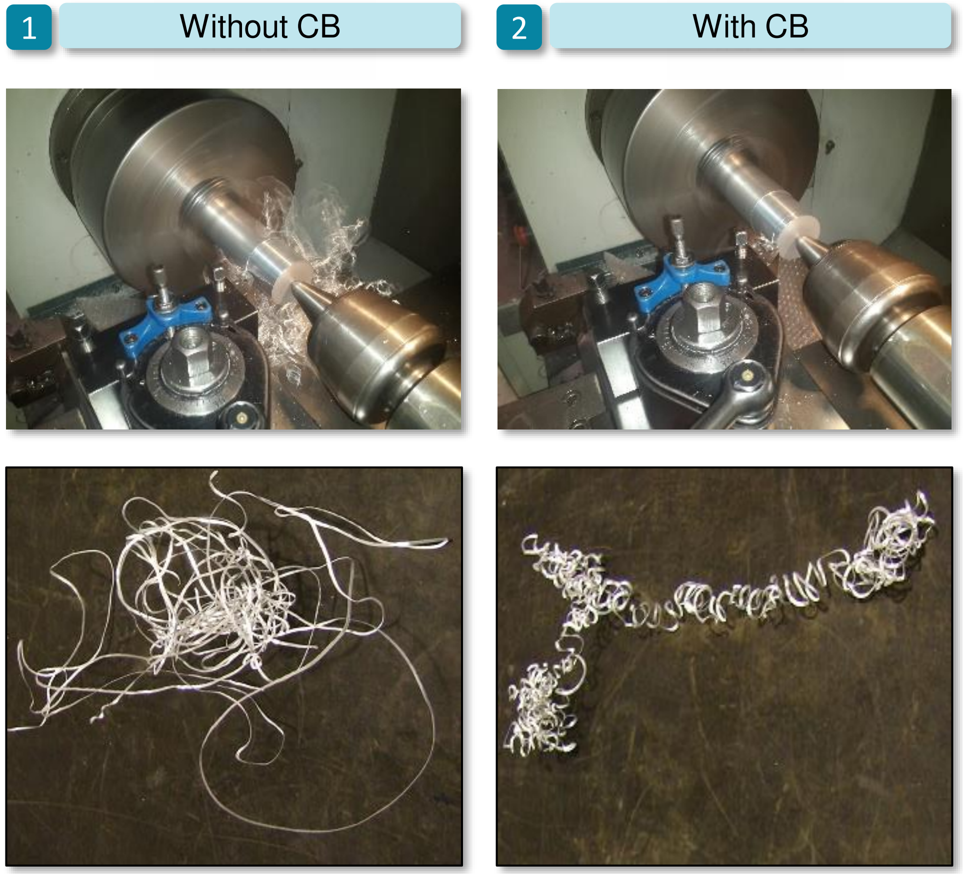
Objective: Design of chip-breakers geometry by FEM simulation

Modelling Tool: Advantage



Cutting force = 197.4 N
Temp = 198,7 ºC

Cutting force = 124.5 N
Temp = 170.6 ºC



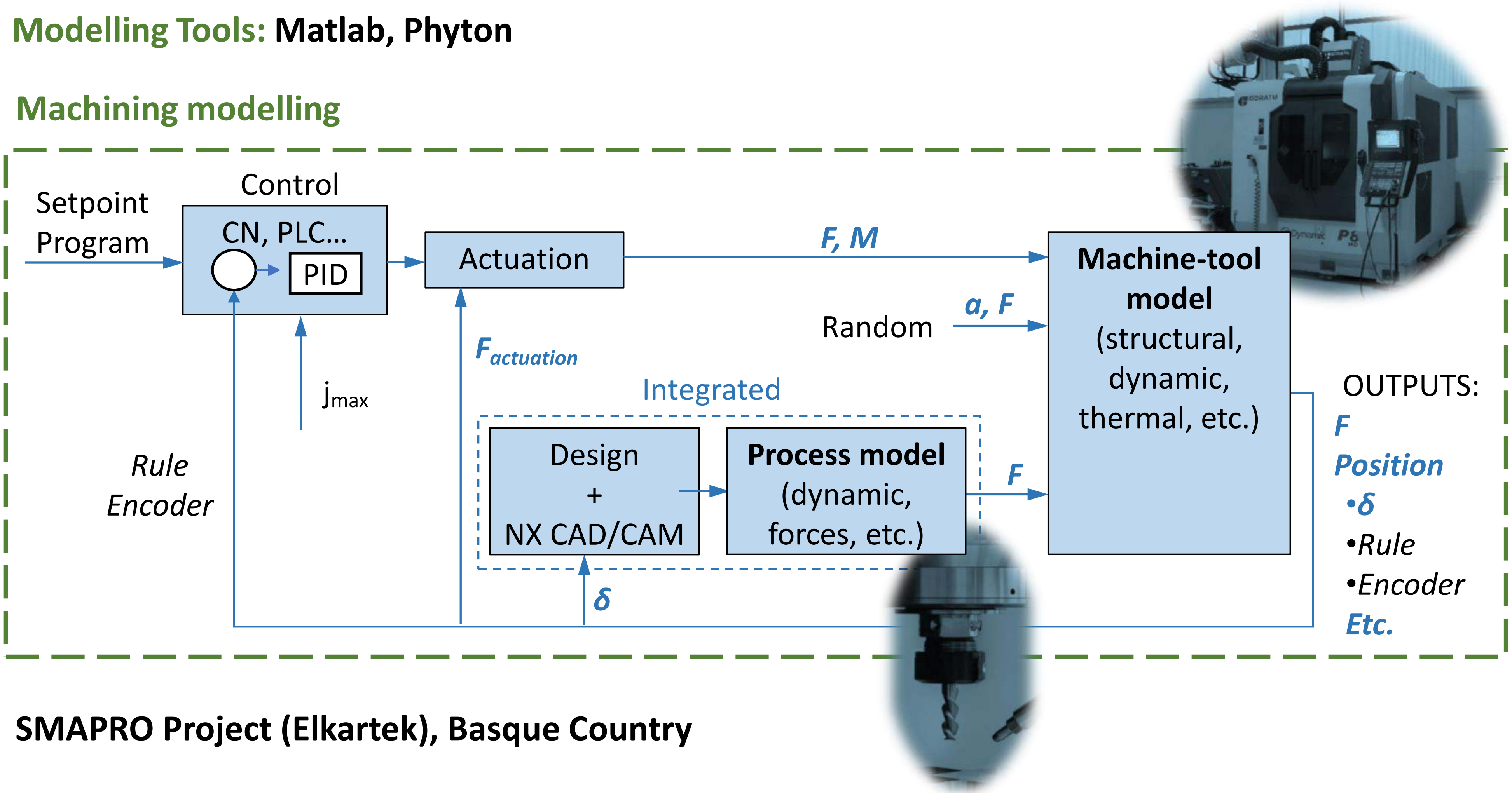
Turning of ductile materials (i.e. aluminium)

+ Laser Additive manufacturing of the chip-breaker

Process Optimization: Model integration & control

Modelling Tools: Matlab, Phyton

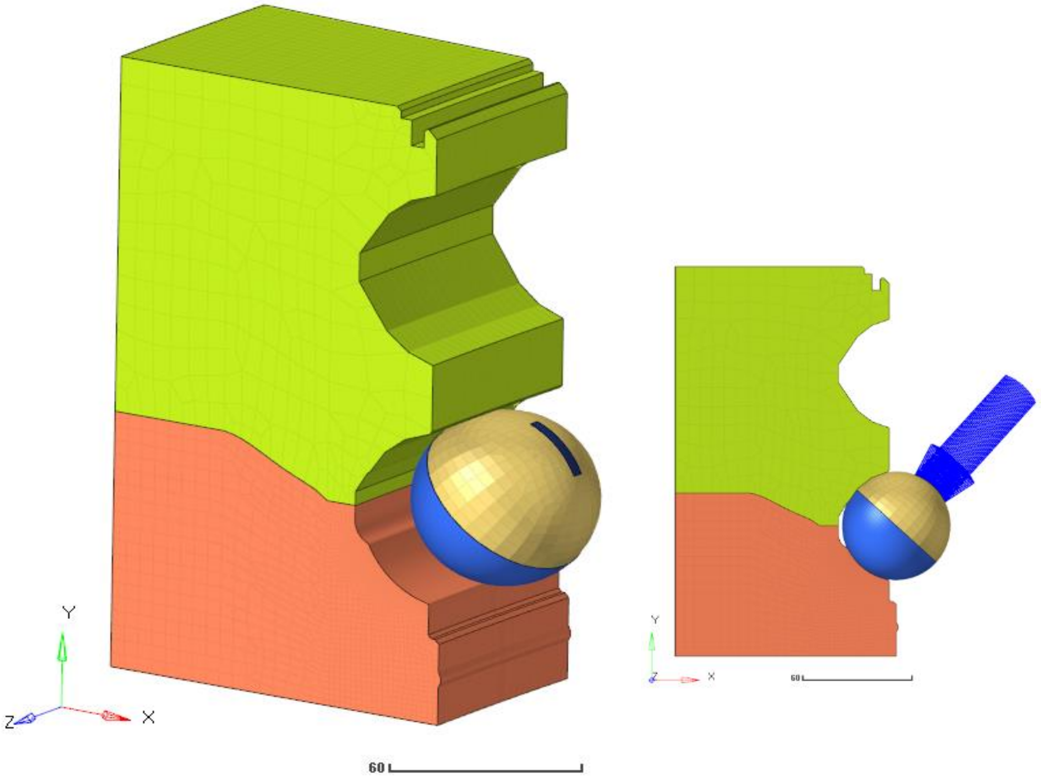
Machining modelling

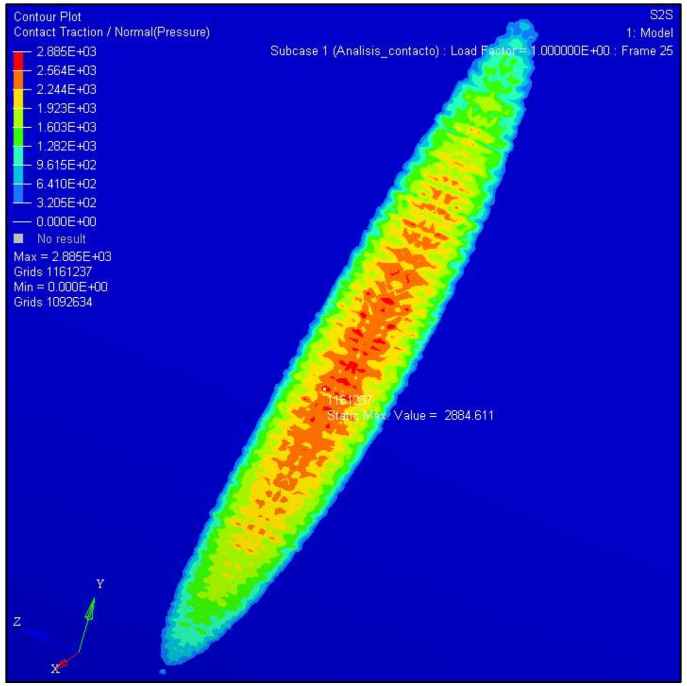


SMAPRO Project (Elkartek), Basque Country

Performance Optimization: Modelling Ball Bearings

- Modelling tools (FEMS, KISSsoft, BEARINX)
- Calculation of the **contact pressure**, useful for the **prediction of different failures:** Rolling contact fatigue, false brinelling… (analytical formulas)





Performance Optimization: Moulds (plastic and metal injection)

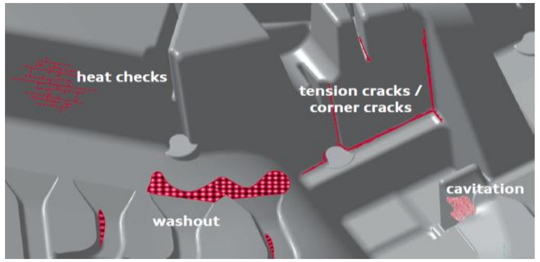
MODELING MOLD WEAR PERFORMANCE

THE FAILURE MECHANISM

- Thermal Fatigue
- Die Soldering
- Erosion
- Abrasion
- Corrosion

High Pressure Die Casting: Thermal Fatigue, Die Soldering, Erosion

Plastic Injection Molding: Erosion, Abrasion, Corrosion



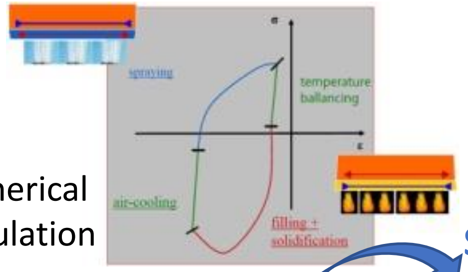
THE NEED

Example of Durability needs:
100-300.000 castings
Real durability:
5000-25000 cycles
Substitution cost of mold insert: 50000€
Shutdown cost/day: 3000€

Financed by EU Commission Project Music: FoF-ICT-2011.7.1
Smart Factories: Energy-aware, agile manufacturing and customization

Performance Optimization: Modelling thermal fatigue

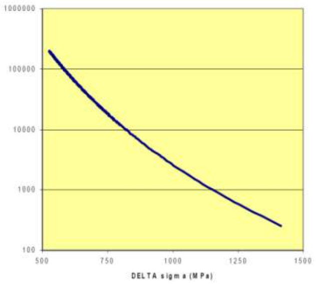
Numerical calculation



Stress

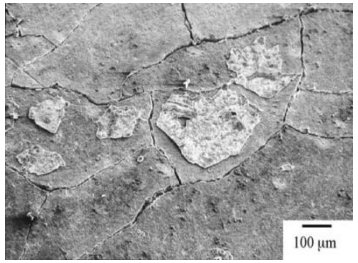
Fatigue uniaxial tests

Temp Gradient ΔT



Cycles N

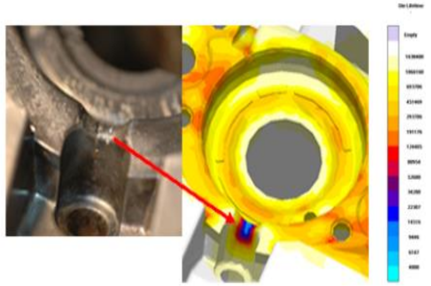
N (cycles) = f (Δσ)

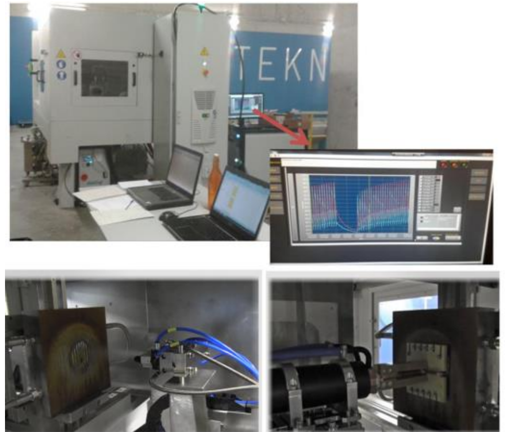


Influence:
- *Material properties*
- Thermal stresses
- Stress concentrators

Cycles to Failure

Thermal Fatigue Test bench





Temperature

N (cycles) = f (T°C)

Crack Initiation Prediction

Software Validation

Performance Optimization: Wear Model Implementation HPDC

HPDC Example:

Thermal Fatigue

N (cycles) = f (stress)

Where

S: thermal stress calculated (820-920 MPa)

Die Soldering

N(cycles)= f (Temperature, pressure)

Where:

T: *Mould surface temperature* (350 - 450ºC)

P: *Pressure in the mould surface* (0 - 7 MPa),

K: *depending on lubricant*

Erosion

Wear(µm/h)=f (angle, speed, hardness)

Where:

VEL: flux speed (32-64m/s)

ANG: impact angle (15-90º)

H: Hardness (200-900HV)

Reference case:

INPUT		
MaxT	400	°C
Thermal stress level	870	MPa
Pressure	1	MPa
Impact speed	50	m/s
Impact angle	30	°
Lubricant	2.68	D
Die material	1	H13

Failure prediction:

OUTPUT		
Thermal Fatigue	7369	Cycles
Die Soldering	956	Cycles
Erosion	17269	Cycles

Improved case:

INPUT		
MaxT	400	°C
Thermal stress level	820	MPa
Pressure	1	MPa
Impact speed	40	m/s
Impact angle	30	°
Lubricant	1	A
Die material	1	H13

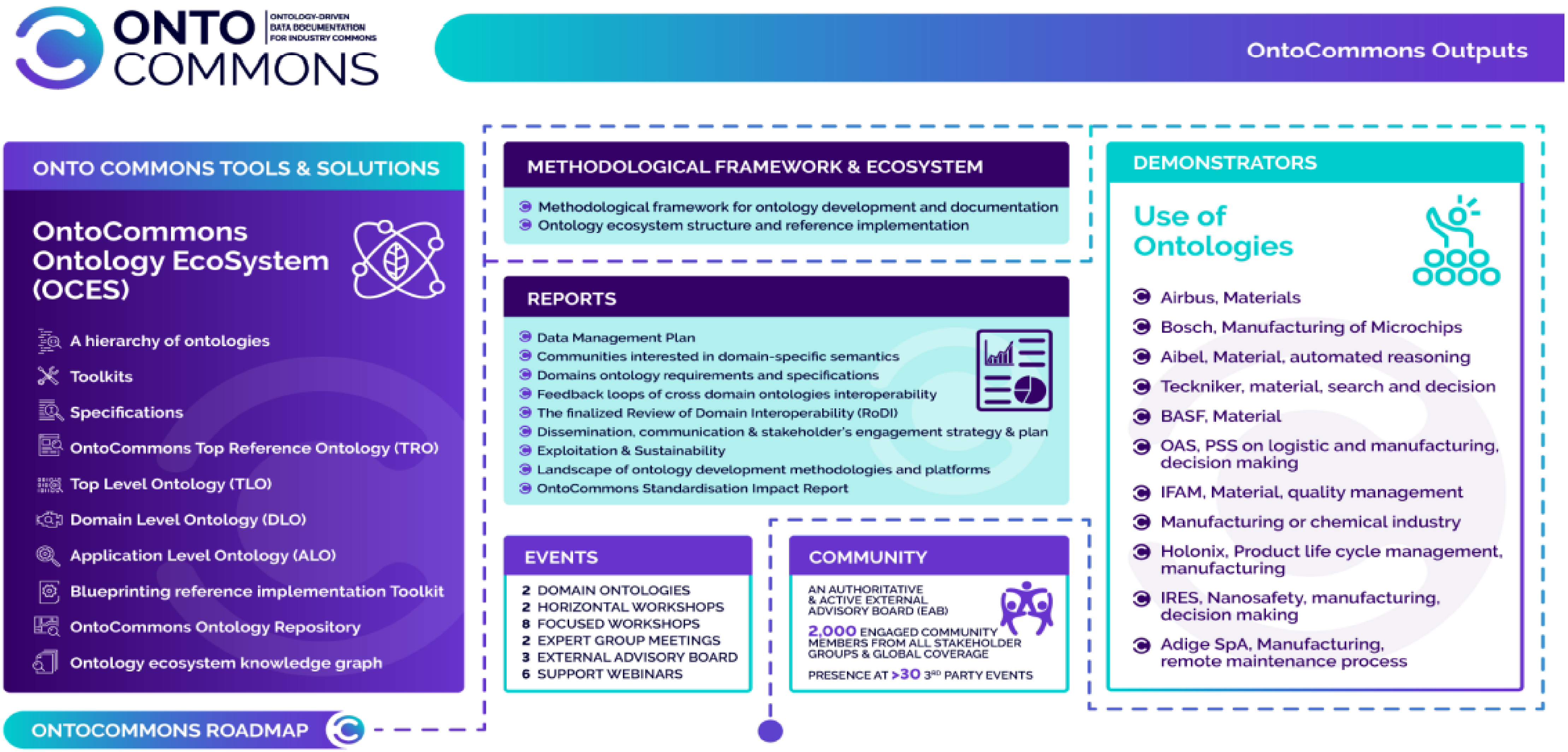
Failure prediction:

OUTPUT		
Thermal Fatigue	**18026**	**Cycles**
Die Soldering	**11286**	**Cycles**
Erosion	**30698**	**Cycles**

time for mould reparation x 2

time for maintenance stops x 10

Ontologies, Onto Commons Project



OntoCommons Stakeholder Groups

- **Scientific communities** in materials, chemistry, nanosafety, characterisation and manufacturing (e.g. NIST, IFAC TC5.3, IEEE, etc.)
- **Ontologists** in these fields (e.g. NCOR, and via IOF, RDA etc.)
- Materials and manufacturing **industries** (e.g. FIAT, DNV-GL, Total, SIEMENS, ABB, etc.)
- Associations and working groups in **ontologies** (IAOA, IOF, eCl@ss, ETSI-SAREF, etc.)
- Associations and working groups in **materials** (e.g. EMMC, EMCC, EUMAT, FAIR-DI, EPPN, Nanosafety Cluster)
- Associations and working groups in **data science** (e.g. RDA, EUDAT, BDVA, International Data Spaces Association)
- Associations and working groups in **manufacturing** (EFFRA, AIOTI, Intelligent Manufacturing Systems (IMS), plattform-i40, IOTA Foundation, ONEM2M, etc.)
- **Standards committees** (e.g. W3C, ISO/IEC JTC1, ISO/TC 184, IUPAC etc.)

See the video (ES)

If you would like to be part of OntoComons external expert Group: Home | OntoCommons.eu

CONCLUSIONS

The use of modelling to:

- Molecular Dynamic and Atomistic modelling to predict **properties at the nanoscale**
- **Piezoelectric simulation** has been used for product (nebulizer) design
- Optimization of **laser and curing processing** by modelling
- **Machining models** to improve the process, reduce the experimental set-up
- **New tool geometries** to reduce manufacturing errors.
- Use **FEM tools** to **predict failure** modes analytically and define tribological tests
- Prediction failure modes lifetime: constructing innovative equipment's, reproducing wear mechanisms, **building lifetime equations from experimental data**
- **Use a common ontology for modelling and data acquisition (OntoCommons)**
- **If you are interested in EMMC or OntoCommons, please tell us.**
- **Contact: Amaya Igartua (amaya.igartua@tekniker.es)**

ACKNOWLEDGEMENTS

EU Commission for financing, POCO, NANOPIGMY, PM JOIN, SPARTA, MUSIC, ONTOCOMMONS and BASQUE COUNTRY for financing the projects, EMACOMP, ELKARTEK, EMAITEK

European Commission

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Agencia Vasca de la Innovación