Advances in multi-scale modelling approaches of liquid metals and alloys for advanced nuclear applications

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Reunión Española de
"**Modelado, caracterización y desarrollo de aleaciones metálicas para aplicaciones nucleares**"
Madrid, 27-28 de Febrero de 2019

1. ABOUT ICAMCyL

2. ICAMCyL & MATERIALS DISCOVERY

3. PREVIOUS PROJECTS

4. CURRENT PROJECTS

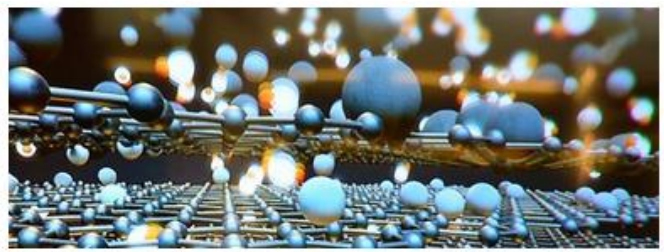
ICAMCyL, A REFERENCE COMPETENCE CENTER

Non-profit private **research foundation** and **competence center**, founded by some of the main industries from the CyL region in the sectors of advanced materials, engineering, mining and processing and automotive, with the support of the regional government of Castilla y León and the County Government of León.

Key player in the European strategy for the efficient management of industrial resources, energy efficiency, eco-innovation and substitution of critical raw materials with the aim of **promoting the development** of advanced materials for the regional network of industries and the **valorization** of the Castilla y León richness in raw materials, in line with its **Smart and Intelligent Specialization Strategy** (**RIS3**).

SUSTAINABLE MINING

The development of a sustainable and low environmental impact 21st century mining through the development and integration of novel methods, techniques and processes that allow the utilisation and valorisation of raw materials and subproducts, always in agreement with the principles of sustainability and circular economy.



ADVANCED MATERIALS

The development, preparation and fabrication of the last generation novel advanced materials with high added-value, and their application in products and relevant industrial processes. We can highlight nanomaterials like polymers, composites or carbon-derived (graphite, graphene); ceramic materials, materials for additive manufacturing and 3D printing, waste and industrial subproducts, and materials for energy (batteries, fuel cells and gas storage)

TRESCA ENGINEERING SOLUTIONS

telice TECHNOLOGY IN THE FIELD

tvitec

Bench & Ground

PEAL

INTAUXMA

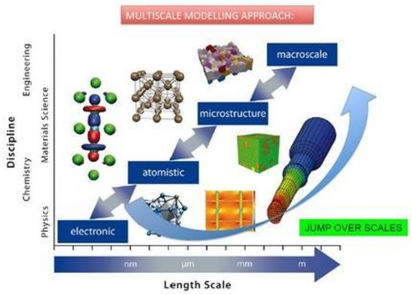
DIPUTACIÓN DE LEÓN

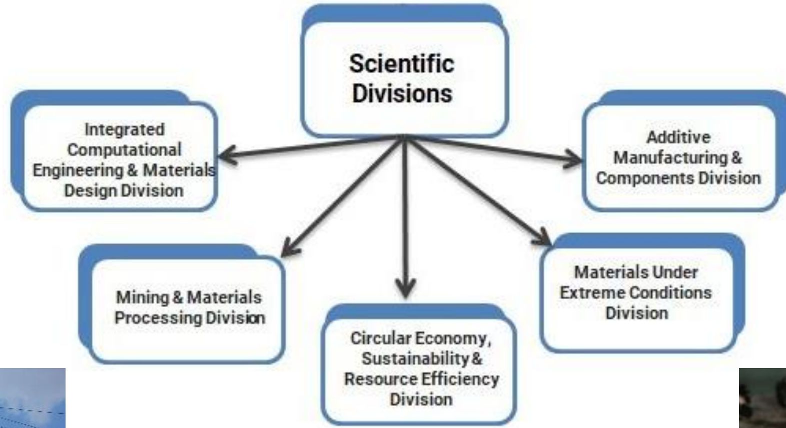
fsb fundaciónsantabárbara

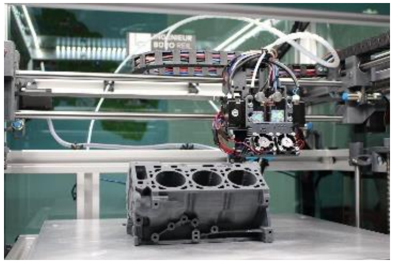
Junta de Castilla y León

competitividad empresarial ice

ICAMCyL, A REFERENCE COMPETENCE CENTER







ADVANCED MINING TECHNOLOGIES

- Exploration
- Classification
- Processing

CIRCULAR ECONOMY

- Waste
- Recycling
- Valorisation

SUSTAINABILITY

- New production methods
- Eco-innovation
- Resource efficiency

NANOMATERIALS

- Carbon-based
- MOFs
- Composites
- Alloys

FABRICATION

- Additive manufacturing
- Pilot lines
- Industry

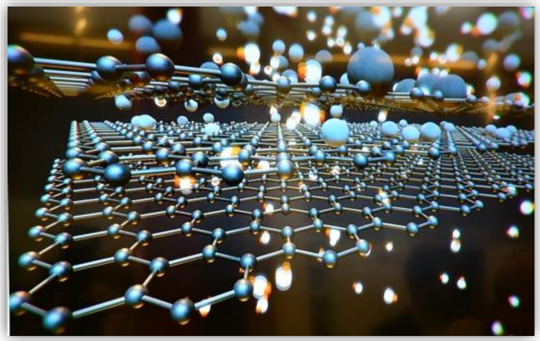
ENERGY & CLIMATE CHANGE

- Batteries /fuel-cells
- CO_2 capture
- Smart cities

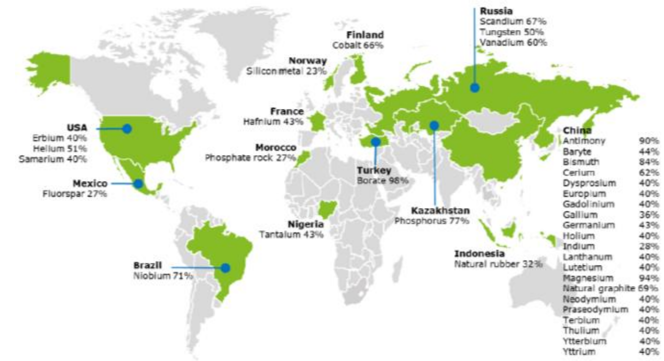
POLES OF INNOVATION

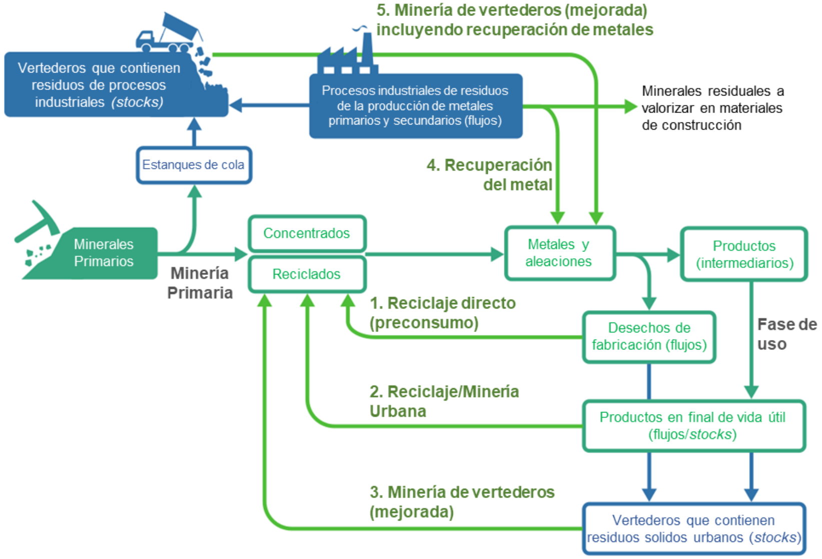
POLO PARA LA INNOVACIÓN DEL CARBÓN(O): RECUPERACIÓN DE LAS CUENCAS MINERAS MEDIANTE LA PRODUCCIÓN DE MATERIALES TECNOLÓGICOS DE BASE CARBONO A PARTIR DEL CARBÓN

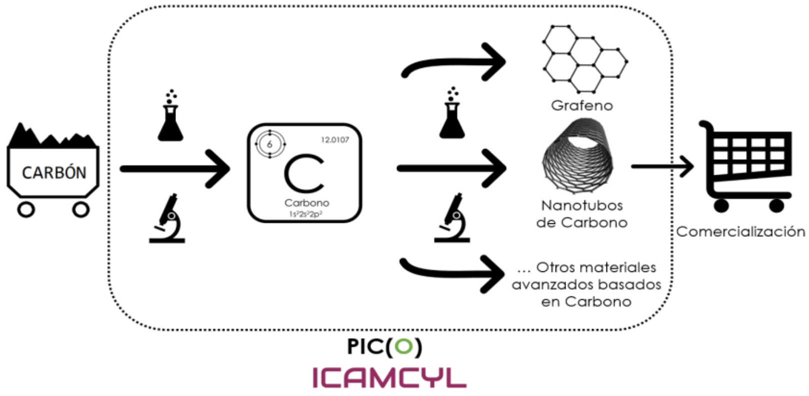
POLO DE INNOVACVIÓN Y RESTRUCTURACIÓN SOCIAL DE LAS CUENCAS MINERAS HACIA UNA NUEVA MINERIA SOSTENIBLE



Revitalizing the CyL region: recovering coal mining places by the creation of an innovation pole for carbon







ICAMCYL

Join the SMART SPECIALISATION PLATFORM

KEMIJSKI INŠTITUT

GRUPO spri TALDEA

METROPOOL REGIO EINDHOVEN

RÉGION Nouvelle-Aquitaine

Junta de Castilla y León

La Région Auvergne-Rhône-Alpes

EMIRI

Agencia Andaluza de la Energía
CONSEJERÍA DE ECONOMÍA, INNOVACIÓN Y CIENCIA

Advanced materials for batteries

ELECTRO MOBILITY | **STATIONARY ENERGY STORAGE**

Aim of this S3P – Industrial Modernization is to **bridge the large gap** between research and industrial applications.

ICAMCYL

CURRENT ONGOING PROJECTS

NEXTOWER
Advanced materials solutions for next generation CSP tower systems

MIREU
Mining and Metallurgy Regions of EU

tarantula
Recovery of Tungsten, Niobium and Tantalum occurring as by-products in mining and processing waste streams

European Commission | Horizon 2020 European Union funding for Research & Innovation

EXPLOREMAT: Descubrimiento de materiales avanzados por métodos computacionales para la industria de Castilla y León

VALUECyL: Valorización de las materias primas de los residuos de la actividad minera en Castilla y León

competitividad empresarial ice

Junta de Castilla y León

extreme CRM
Solutions for Critical Raw Materials Under Extreme Conditions

MINEA
Mining the European Anthroposphere

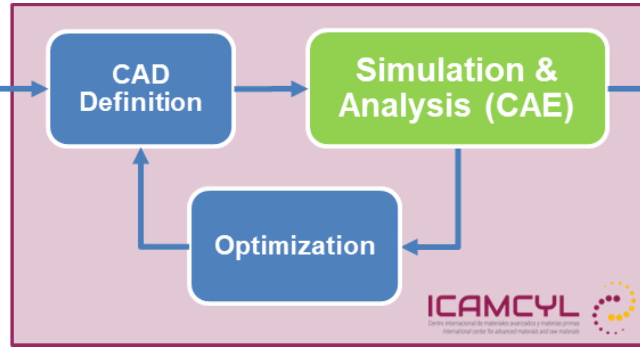
ENGAGER ENERGY POVERTY ACTION
European Energy Poverty: Agenda Co-Creation and Knowledge Innovation

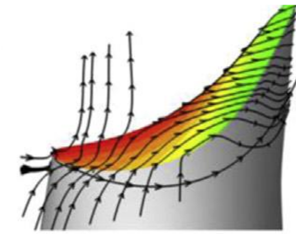
cost EUROPEAN COOPERATION IN SCIENCE AND TECHNOLOGY

eit | European Institute of Innovation & Technology

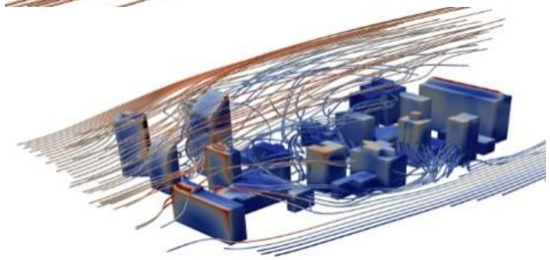
INNOCAT: Innovative CRM substitution technology

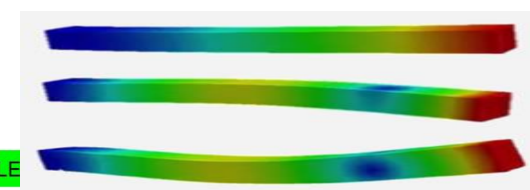
ENGINEERING & MATERIALS DESIGN DIVISION

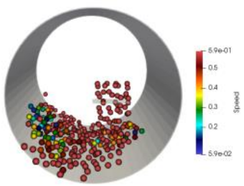


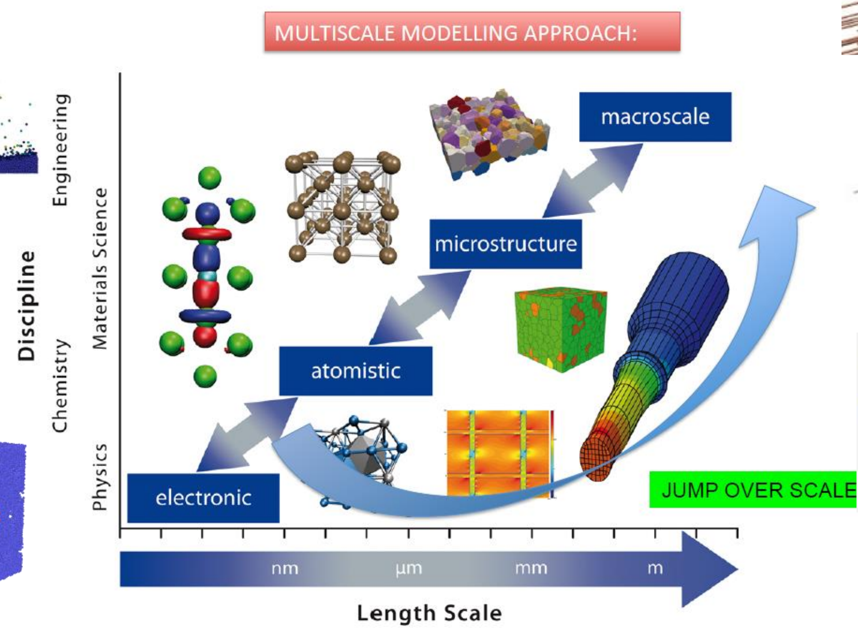


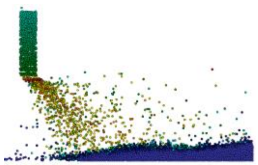
MULTISCALE (DFT, MD, Coarse Grain, DEM)
AbInit, LAMMPS, LIGGGHTS etc

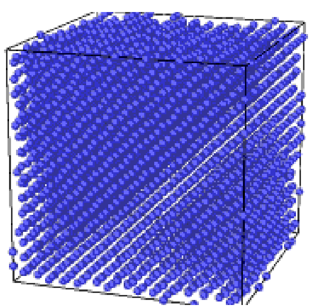


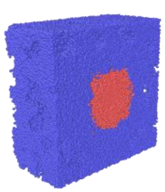


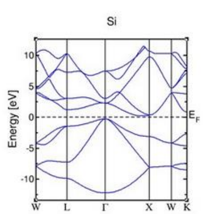












CFD / FEM
Ansys, openFOAM, Salome, etc.

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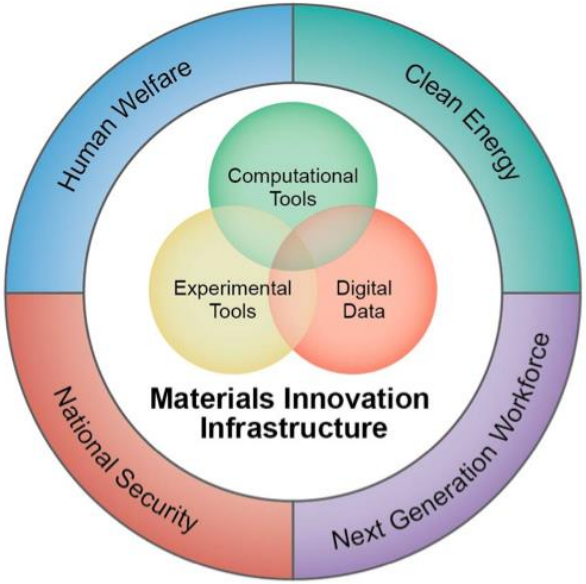
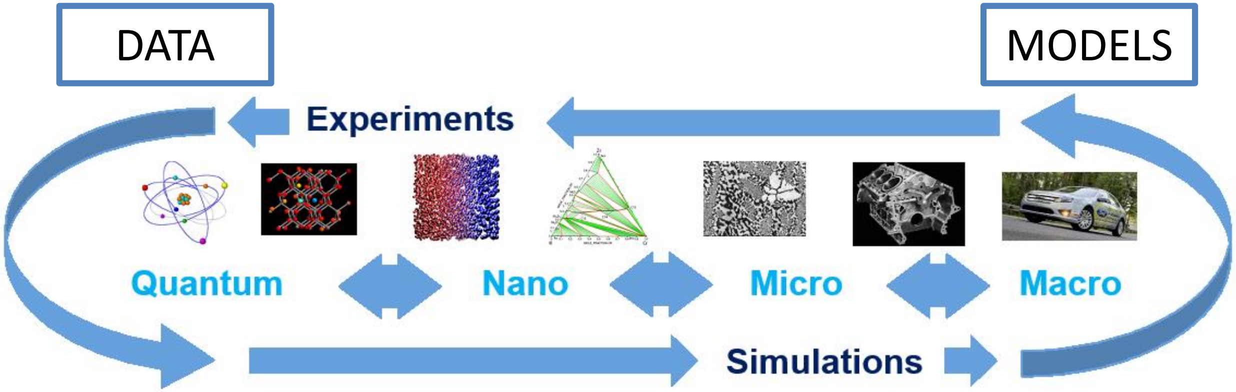
Materials Genome Initiative





TAILORED MATERIALS

1. ABOUT ICAMCyL

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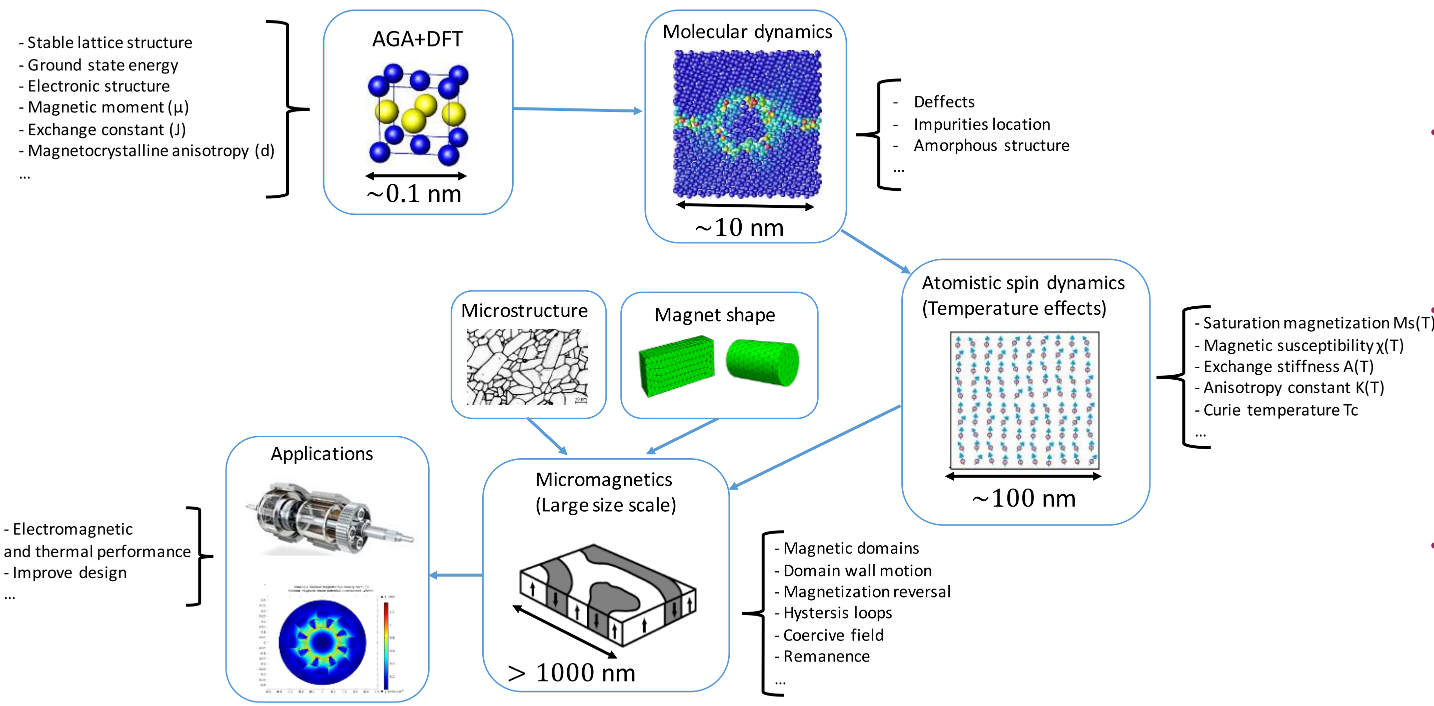
Multi-scale Modelling of Magnetic Materials

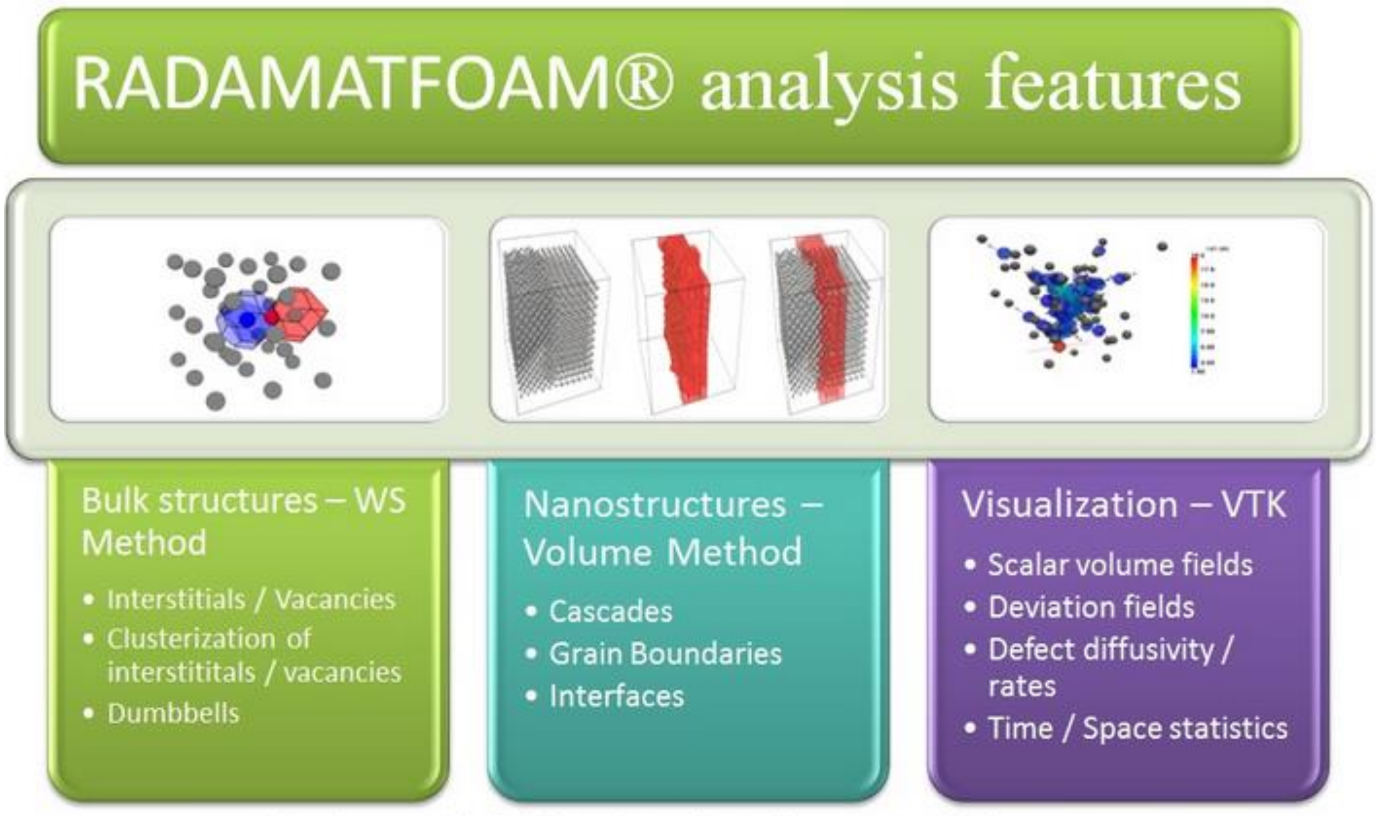
- Applying multiscale techniques to magnetic materials study with adaptative genetic algorithms
- High-throughput exploration of magnetic materials
- From nanostructure to final materials properties
- DFT - > MD -> Coarse Grain -> MacroScale



- Arapan S, Nieves P, Cuesta-López S. *A high-throughput exploration of magnetic materials by using structure predicting methods*. Journal of Applied Physics (2018) 123(8)
- Nieves P, Arapan S, Cuesta-López S; *An adaptive genetic algorithm approach for predicting magnetic structure suitable for high-performance permanent magnet development*; 2017 IEEE International Magnetics Conference, INTERMAG 2017 (2017)
- Nieves P,Arapan S,Cuesta-Lopez S; *Exploring the Crystal Structure Space of CoFe<inf>2</inf>P by Using Adaptive Genetic Algorithm Methods*; IEEE Transactions on Magnetics (2017) 53(11)

Tool for radiation damage in materials

- Software tool base on the open source tool for Computational Fluid Dynamics (CFD) tool OpenFOAM
- Analysis of crystallographic structures in materials under radiation damage

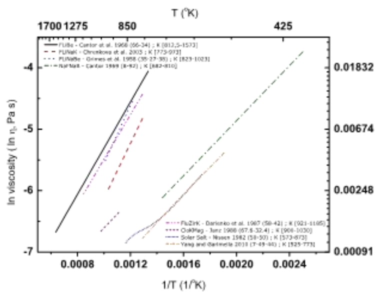


MATFOAM®. Ekhi Arroyo, Jordi Fradera, Santiago Cuesta, UBU. BU-90-12 11/07/2012.

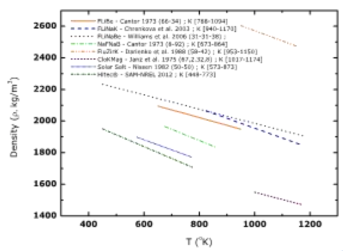
RADAMAT-FOAM® ***Radiation Damage In Materials For Openfoam***. E. Arroyo, J.Fradera, S. Cuesta, U. Burgos. BU 59-13. 03/05/2013.

Database for molten salt properties

Intensive Review



SCATERING, LACK OF DATA




ELSEVIER

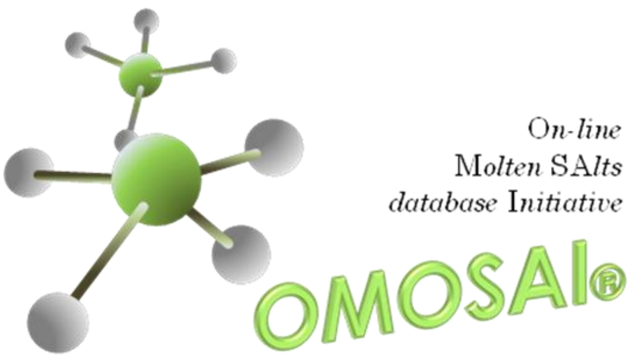
Chemical Engineering and Processing: Process Intensification

Volume 73, November 2013, Pages 87–102

Molten salts database for energy applications

R. Serrano-López, J. Fradera, S. Cuesta-López

Universidad de Burgos, Science and Technology Park, I+D+I Building, Room 63, Plaza Misael Bañuelos s/n, 09001 Burgos, Spain



Friendly web interface

14 Molten Salts
5 Properties

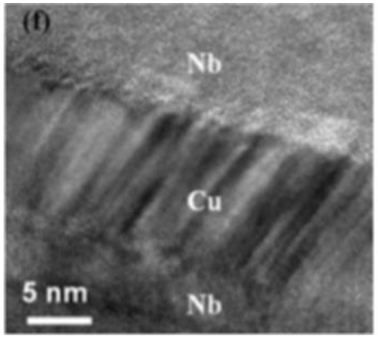
Quick access to data and references by filtering

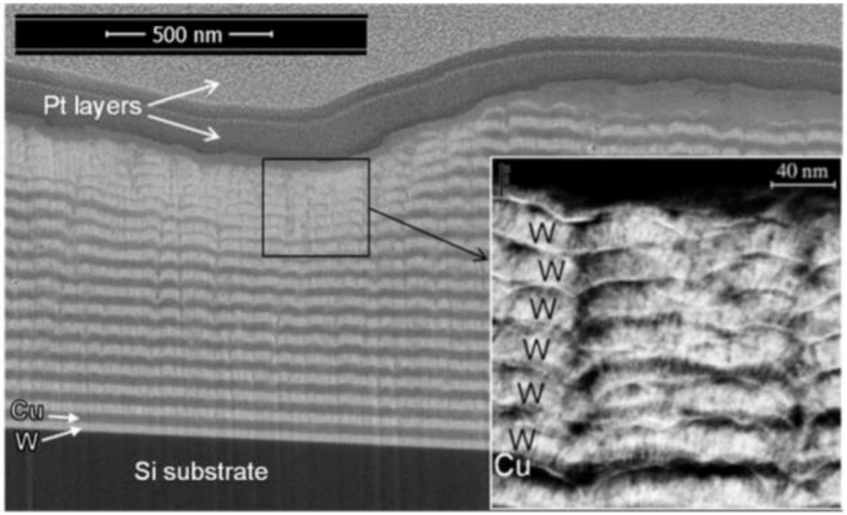
+ Properties prediction section
+ Uncertainties section
…

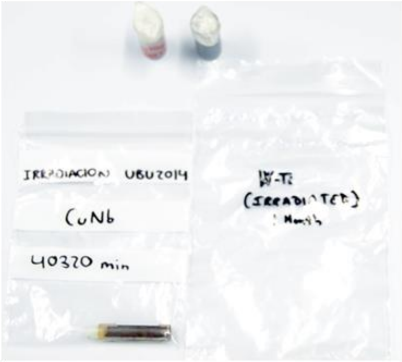
ICAMCYL

From nano to multiscale damage in materials

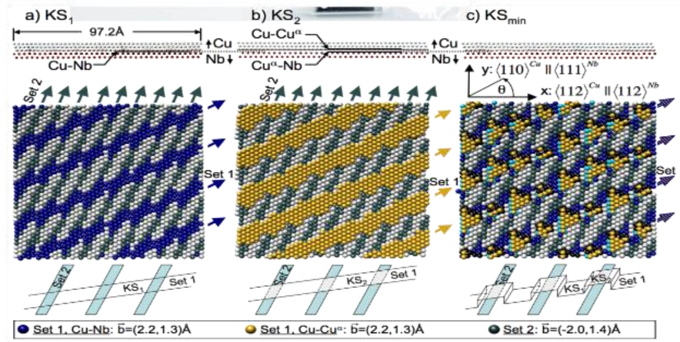
- Nanostructured metallic multilayers
- Radiation damage healing and helium trapping properties
- Objective: changing the life-time perspective of radiation shielding
- CuNb & CuW look stable and arise as solid candidates to form multilayers, nano-structured metallic interfaces







IN COOPERATION with University of Cagliari (F. DELOGU et al)



Source: M. J. Demkowicz, PRL 100, 136102 (2008)

From nano to multiscale damage in materials

He DYNAMICS AT THE INTERFACE

CuNb Interface structure / dynamic information
Anticipation of KS1' structure

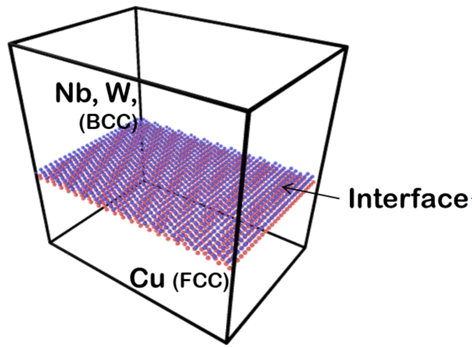
Massive simulations of radiation damage cascades on Cu, Nb, W interfaces -> statistics

STADISTICS OF DEFECTS, DIFUSION COEFICIENTS
IN FUCTION OF ENERGY, PARTICLE, TIME

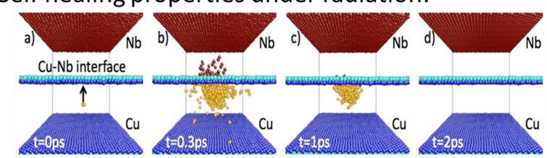
MODEL OF PREDICTION OF DAMAGE AT THE MACROSCALE
DPA-ENGINEERING DESIGN MACROSCALE

- Ortún-Palacios J, Locci A, Fadda S, Delogu F, Cuesta-López S; *Role of Interface in Multilayered Composites under Irradiation: A Mathematical Investigation*; Advances in Materials Science and Engineering (2017) 2017

- Ortún-Palacios J, Locci A, Delogu F, Cuesta-López S; *Self-healing ability assessment of irradiated multilayered composites: A continuum approach*; Journal of Nuclear Materials (2018) 512 391-406

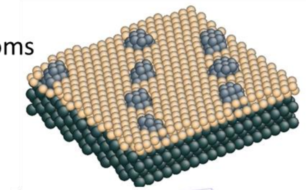


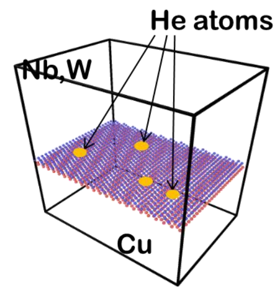
Self healing properties under radiation:

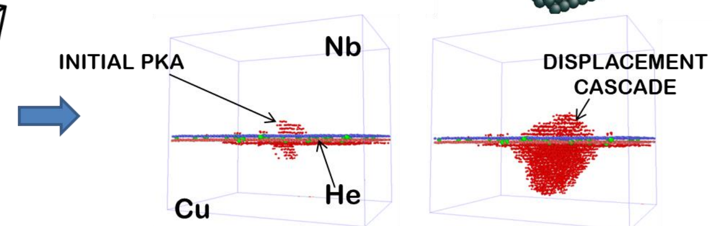


INTERFACE TRAP AND RECOMBINATION OF IRRADIATION-INDUCED DEFECTS

Ability to trap He atoms







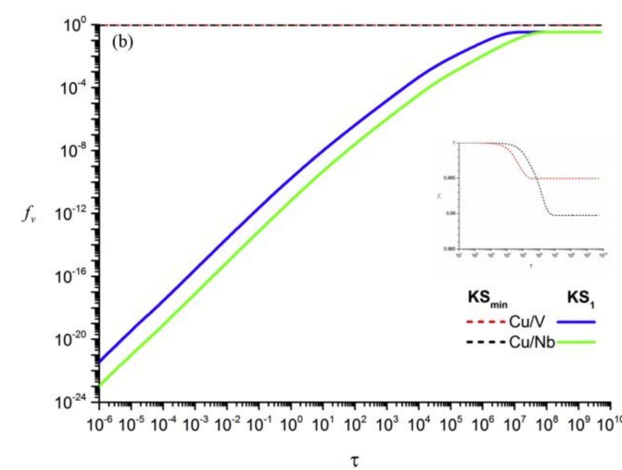
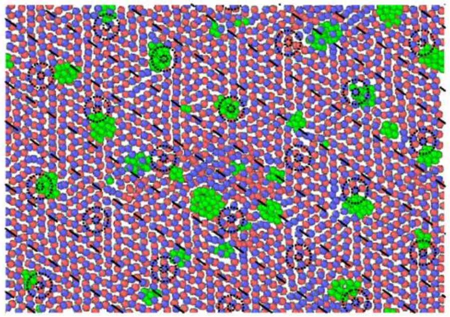


Fig. 9. Temporal profiles of (a) SIA and (b) vacancy trap occupation probability at the interface between metals α and β (z = 1).

From nano to multiscale damage in materials

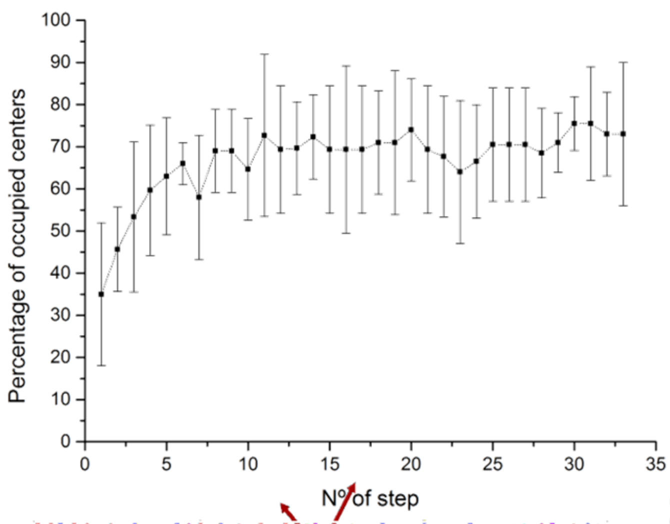
He DYNAMICS AT THE INTERFACE

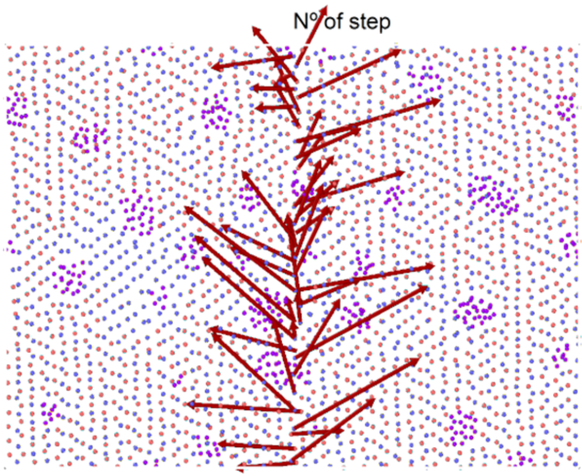


Helium

Copper

Niobium



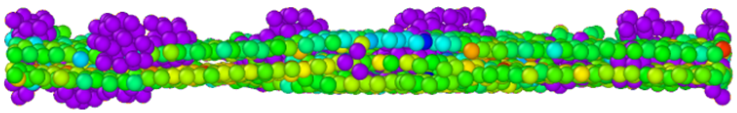


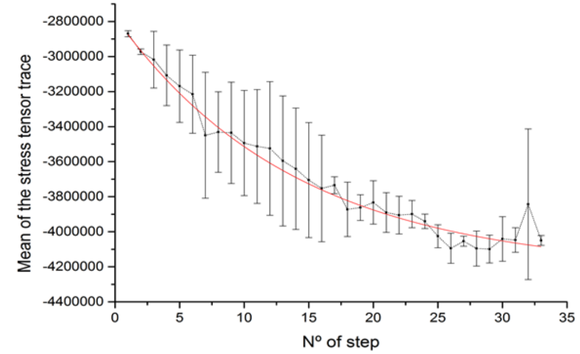
OUR SUCCESS-> WE PROVIDED:

- Confirmation of the existence of a engineering design structural factor relying on the molecular architecture

- A limit in the absorption based on the loose of mechanical properties

- The possibility to predict He confinement/adsorption rates over time





ICAMCYL

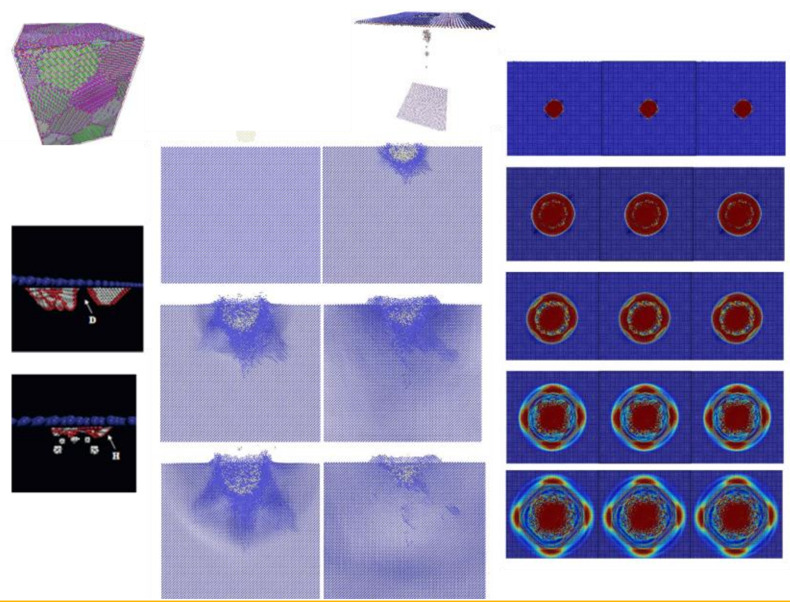
Atomistic view of nano-crashes, nanoindentation and impact phenomena

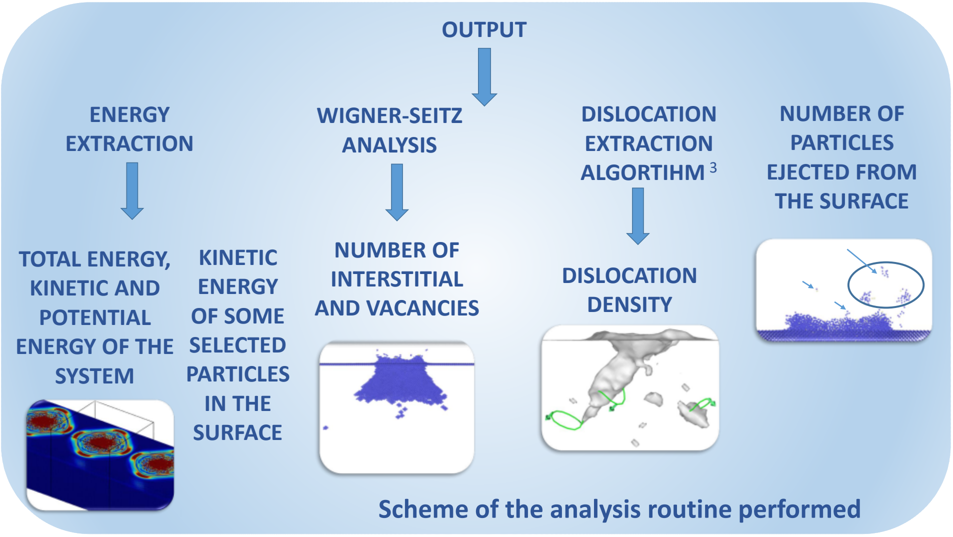
- Refractory materials study: niobium response against the impact of high energy debris
- MD study of microstructure after impact
- Damage response in niobium as shielding material, showing low energy dependence on dislocation density for debries energies over 10 keV
- Methodology can be extended to other refractory metals of industrial interest (tungsten, tantalum)


Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms
Volume 432, 1 October 2018, Pages 24-28

Theoretical study of the performance of refractory materials for extreme conditions applications

Claudia Pecoraro [a, b, c], Santiago Cuesta-López [a, b, c, d]





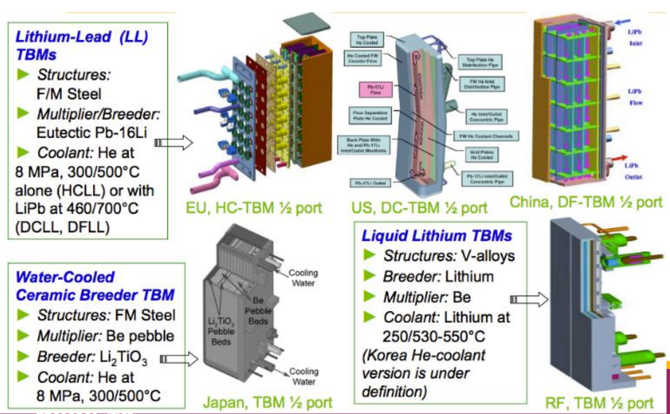
Scheme of the analysis routine performed

Liquid Metals in Nuclear Industry

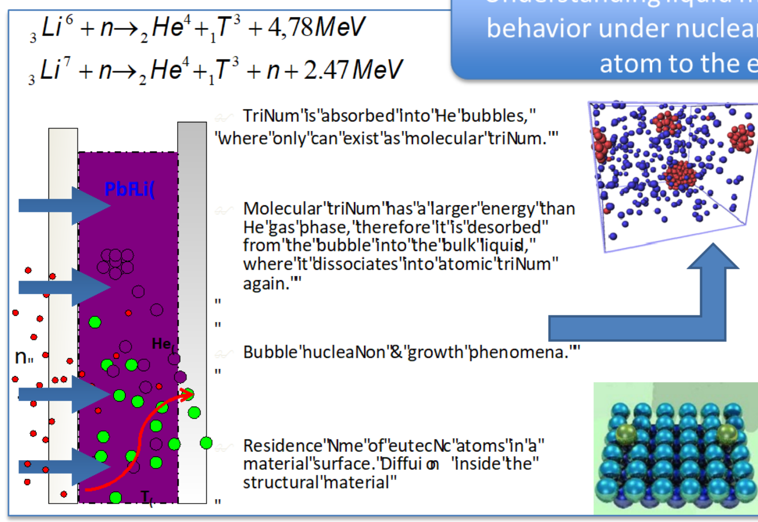
- High relevance of liquid metals as coolants in nuclear industry: ITER project
- Behaviour of liquid metals can be studied with the help of multiscale modelling technique
- Previous experience in this field: developing interatomic potentials for Li-Pb, irradiation effects over coolants.
- Next step: He-Li-Pb interatomic potential

iter

china eu india japan korea russia usa



Understanding liquid metals technology and H+He behavior under nuclear fusion conditions from the atom to the engineering design



POLITÉCNICA

- Fraile, A., Cuesta-López, S., Caro, A., Schwen, D., Manuel Perlado, J. Interatomic potential for the compound- forming Li-Pb liquid alloy (2014) *Journal of Nuclear Materials*, 448 (1-3), pp. 103-108.
- Fradera, J., Cuesta-López, S. Impact of nuclear irradiation on helium bubble nucleation at interfaces in liquid metals coupled to permeation through stainless steels (2014) *Fusion Engineering and Design*, 89 (1), pp. 16-24.
- Fradera, J., Cuesta-López, S. The effect of a micro bubble dispersed gas phase on hydrogen isotope transport in liquid metals under nuclear irradiation (2013) *Fusion Engineering and Design*, 88 (12), pp. 3205-3214.
- Fradera, J., Cuesta-López, S. Nucleation, growth and transport modelling of helium bubbles under nuclear irradiation in lead-lithium with the self-consistent nucleation theory and surface tension corrections (2013) *Fusion Engineering and Design*, 88 (12), pp. 3215-3223.
- Fraile, A., Cuesta-López, S., Iglesias, R., Caro, A., Perlado, J.M. Atomistic molecular point of view for liquid lead and lithium in Nuclear Fusion technology (2013) *Journal of Nuclear Materials*, 440 (1-3), pp. 98-103.

Using CFD technology to make the bridge in design: permeation of helium through fusion steels at interfaces in liquid metals

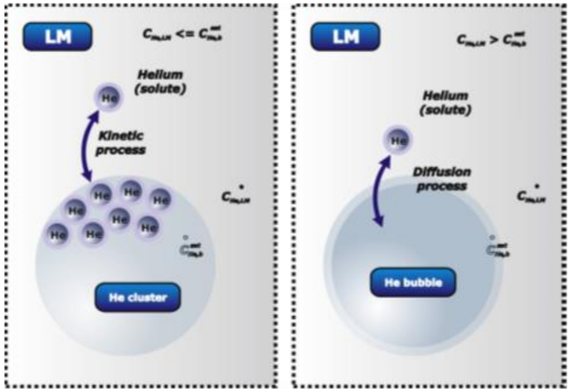


Fig. 1. Kinetic growth model (left) and diffusion growth model (right) showing when a model is used depending on the He concentrations.

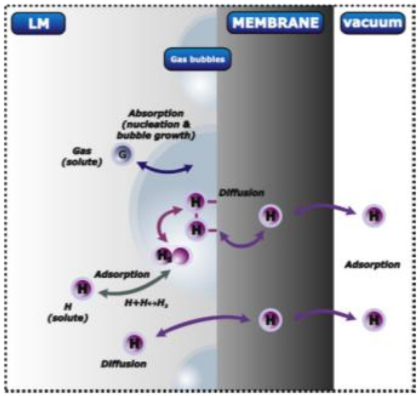


Fig. 1. Hydrogen isotope and helium transport phenomena in a permeation system.

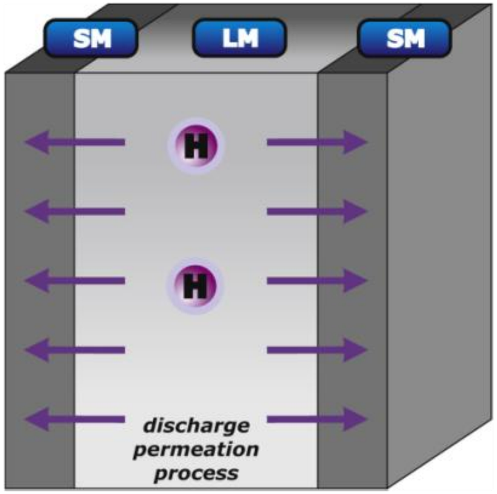


Fig. 3. One dimensional case configuration. Central LLE slab T discharge process through permeation process.

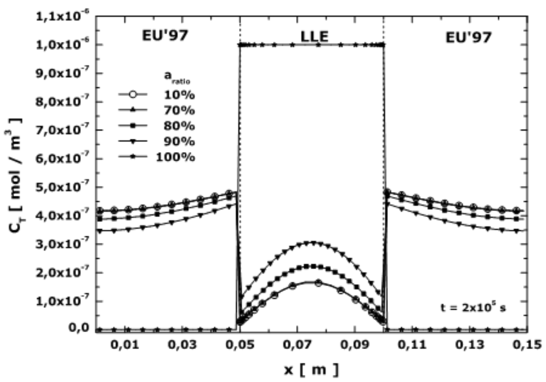


Fig. 8. Concentration profiles at different a_{ratio} for $t = 2 \times 10^5$ s.

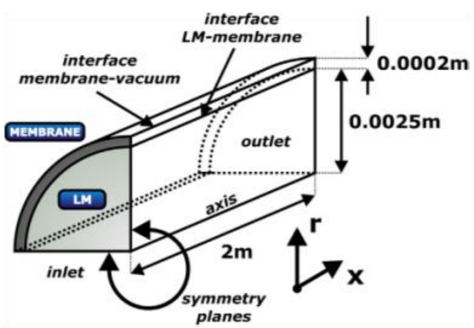


Fig. 9. 3D pipe configuration for the pipe CFD simulation. Symmetry planes are used to save computational resources.

- Fradera, J., Cuesta-López, S. Impact of nuclear irradiation on helium bubble nucleation at interfaces in liquid metals coupled to permeation through stainless steels (2014) *Fusion Engineering and Design*, 89 (1), pp. 16-24.
- Fradera, J., Cuesta-López, S. The effect of a micro bubble dispersed gas phase on hydrogen isotope transport in liquid metals under nuclear irradiation (2013) *Fusion Engineering and Design*, 88 (12), pp. 3205-3214.

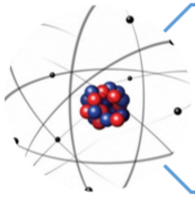
1. ABOUT ICAMCyL

2. ICAMCyL & MATERIALS DISCOVERY

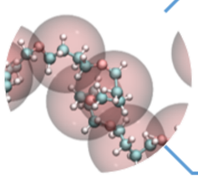
3. PREVIOUS PROJECTS

4. CURRENT PROJECTS

Multiscale modelling of ODS alloys – FeCrAl-Pb interaction

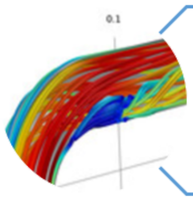


Quantum Molecular Dynamics (QMD) and MD models of materials (Kanthal,FeCrAl Alloys) and coolant (Lead, Lead+Bismuth)



Coarse Grain and Dislocation Dynamics Models of materials (Kanthal,FeCrAl Alloys) and coolant (Lead, Lead+Bismuth)

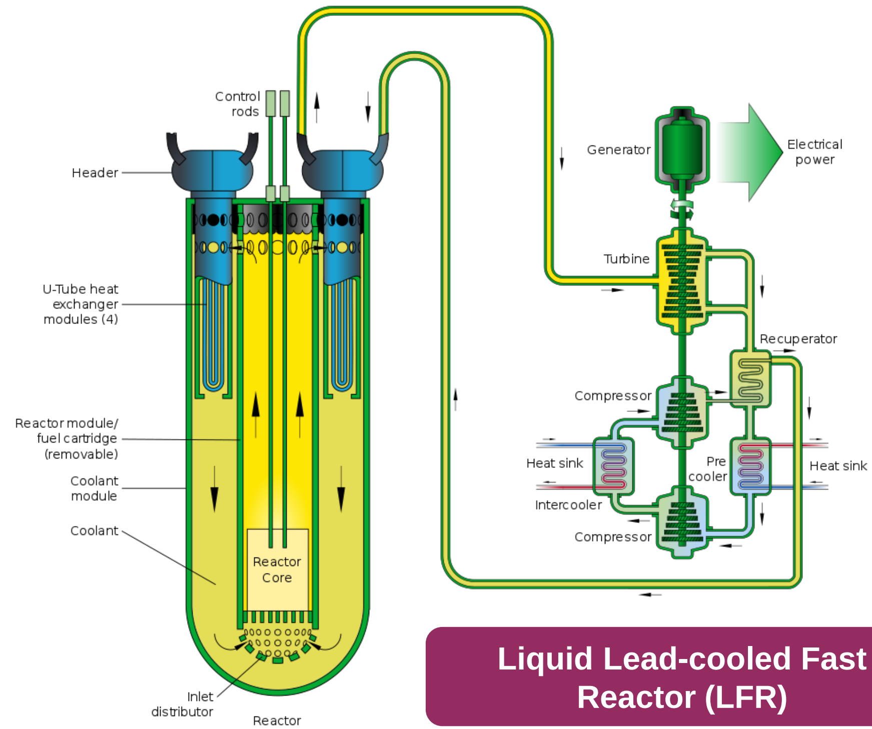
FEED



CFD+FEM modelling of the system under operation conditions

DAMAGE ESTIMATION WITH RESPECT TO MATERIALS COMPOSITION AND WORKING CONDITIONS

LIFE TIME PREDICTION WITH HIGHER PRECISION



Liquid Lead-cooled Fast Reactor (LFR)

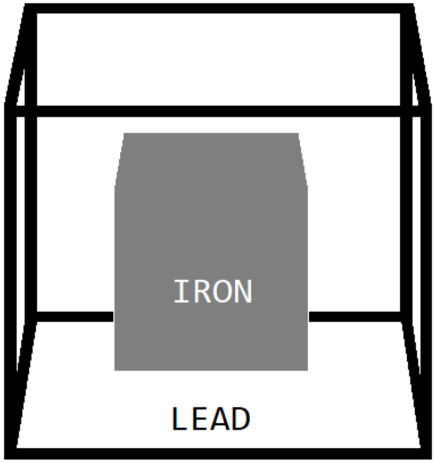
OUR APPROACH

1. MD model for liquid metal corrosion
2. Coupled CFD+FEM model for liquid metal refrigeration

NANOSCALE MODEL: FeCrAl-Pb interaction

Objective:

- FeCrAl-Pb corrosion study
- Pure diffusion approach to corrosion



Steps:

1. Build model with Fe and Pb
2. Study diffusion coefficients dependence with T
3. Build FeCrAl and study diffusion of components
4. Build Alumina and study diffusion

LJ potentials

$$V(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

✓ More elements can be considered

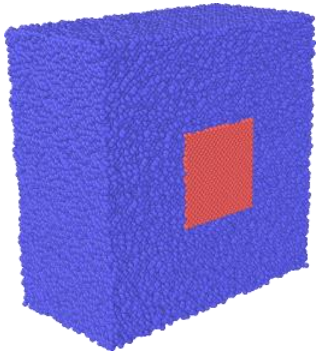
✗ Less accurate

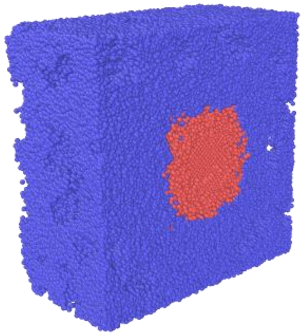
MEAM potentials

$$E_{tot} = \sum_i \left[F_i(\bar{\rho}_i) + \frac{1}{2}\sum_{j(\neq i)} S_{ij}\phi_{ij}(R_{ij})\right]$$

✓ More accurate

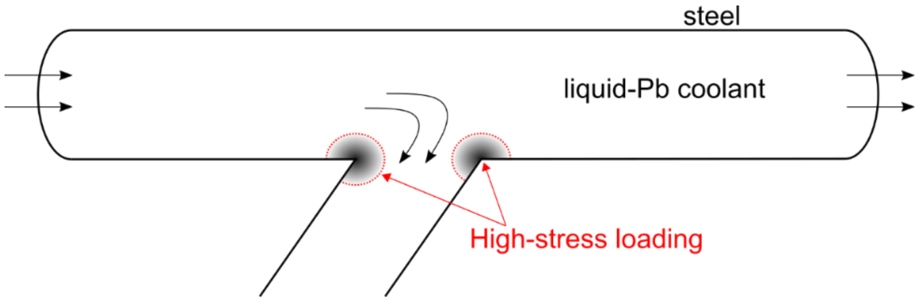
✗ Only available for a few elements

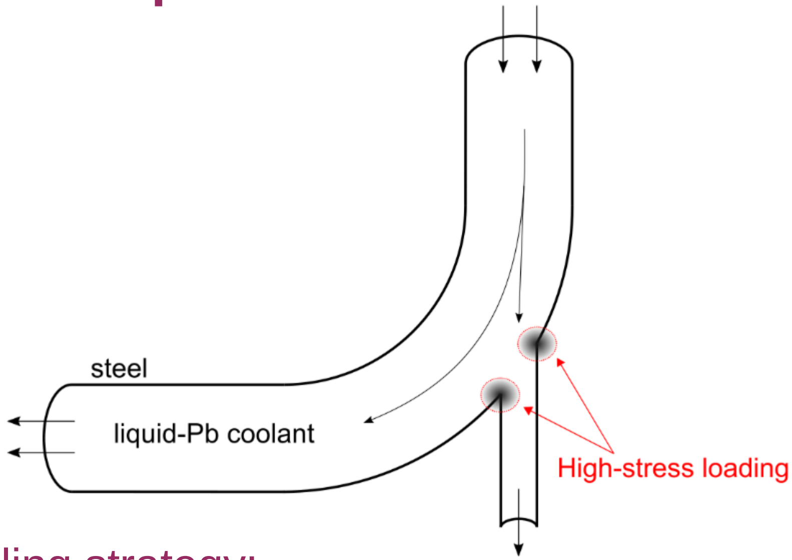


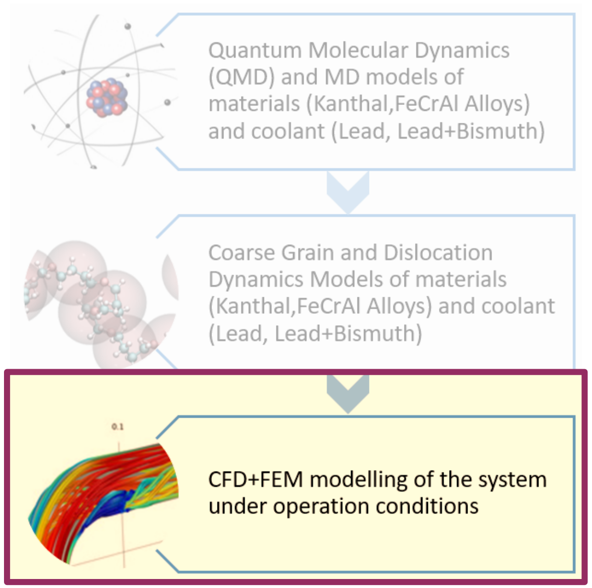


MACROSCALE MODEL: FeCrAl-Pb interaction

The physical problem now at a macros-scale level: **appearance of weak points under long-term operation**





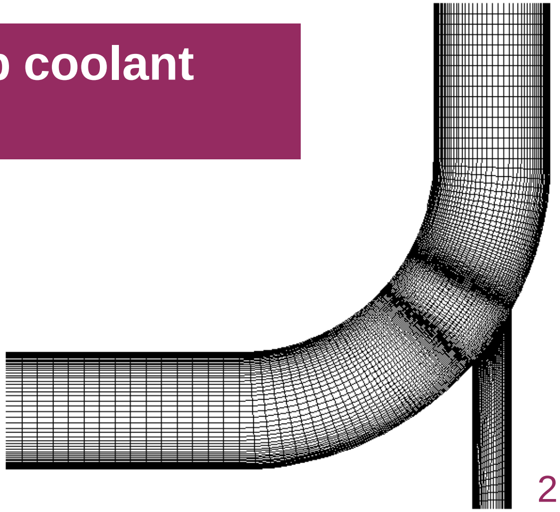


<u>CFD+FEM coupling strategy</u>:

- Interactions between liquid-Pb coolant and Kanthal pipe
- High shear-stress and thermal loading near joints
- How can these additional loads affect the aging and thus the operability of the solid material?
- Steady state vs. Transient operation

MACROSCALE MODEL: FeCrAl-Pb interaction

CFD simulations to investigate the liquid-Pb coolant flow problem



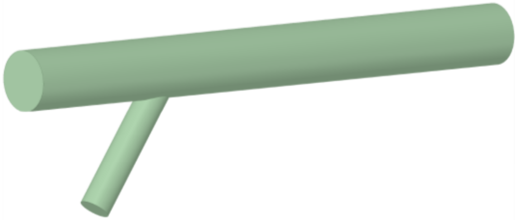
2D mesh

1. Mesh Generation

- Structured grids
- Low y^+ to resolve with enough accuracy hydrodynamic and thermal boundary layer
- Grid sensitivity study

2. Numerical Simulations

- ANSYS Fluent solver (2D + 3D with thickness at later stage)
- Steady state + time-dependent simulations with heat transfer and buoyancy-driven effects
- Realistic internal cooling flow conditions: Reynolds number range $Re_D \in (10^4 - 10^6)$, fully turbulent flow
- Working fluid: pure liquid-Pb (with the possibility to include impurities at a later stage from molecular analysis)

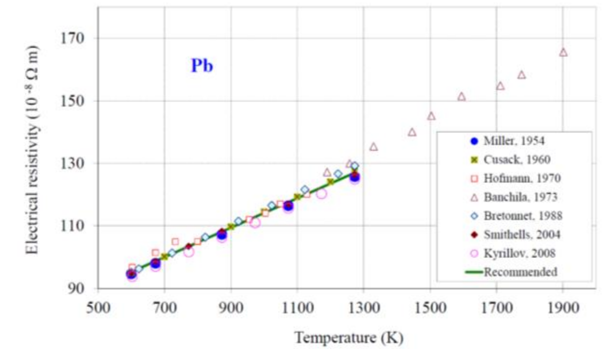


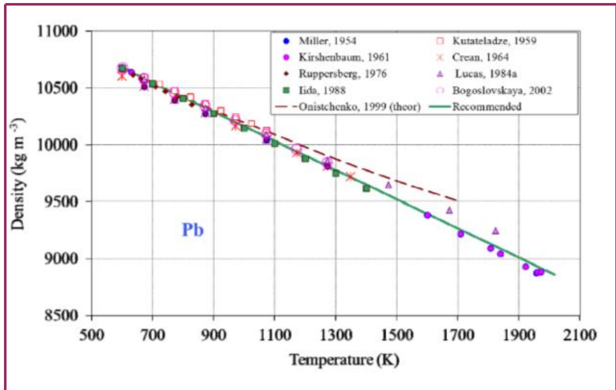
3. Post-processing

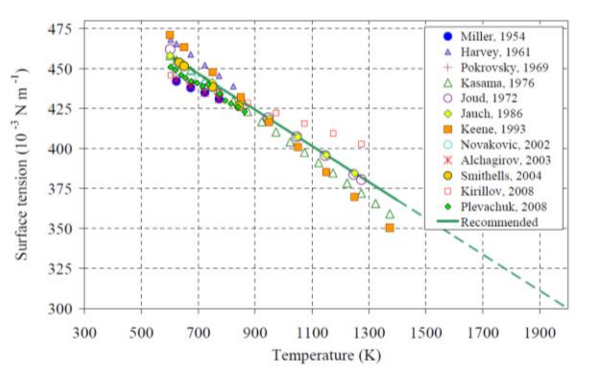
- Wall data regarding shear stress, friction coefficient, heat flux, temperature, among others

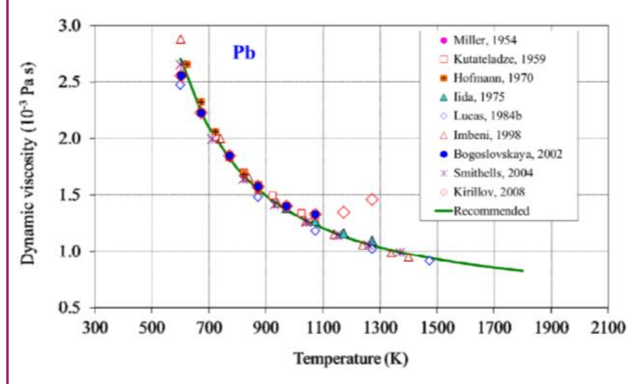
MACROSCALE MODEL: FeCrAl-Pb interaction

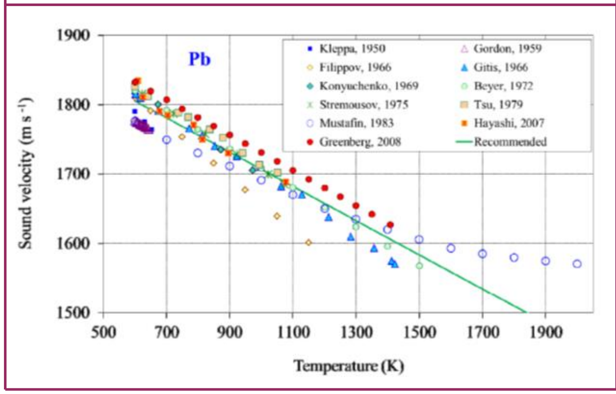
Correlations extracted from:
Vitaly Sobolev, *Database of thermophysical properties of liquid metal coolants for GEN-IV – Sodium, lead, lead-bismuth eutectic (and bismuth)*, Scientific Report SCK-CEN-BLG-1069, Belgian Nuclear Research Centre, 2011.

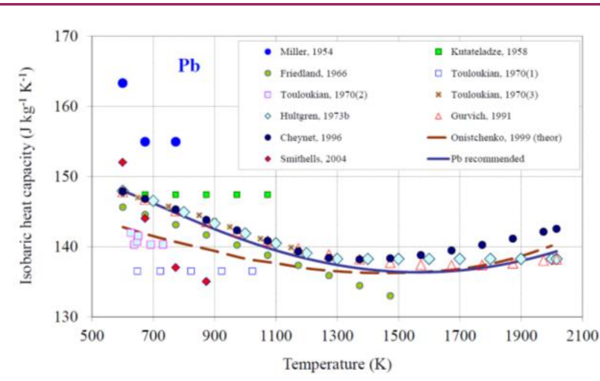


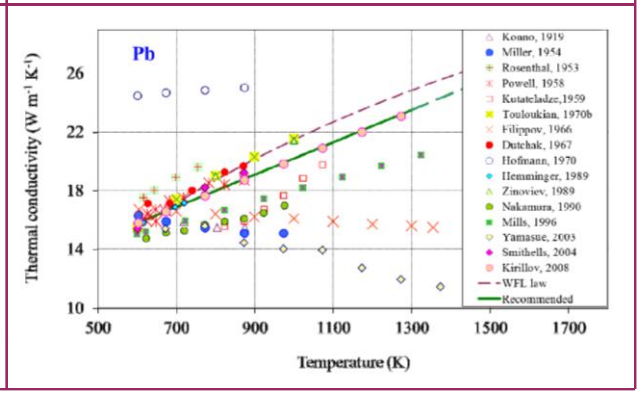












KANTHAL®
Part of Sandvik Group

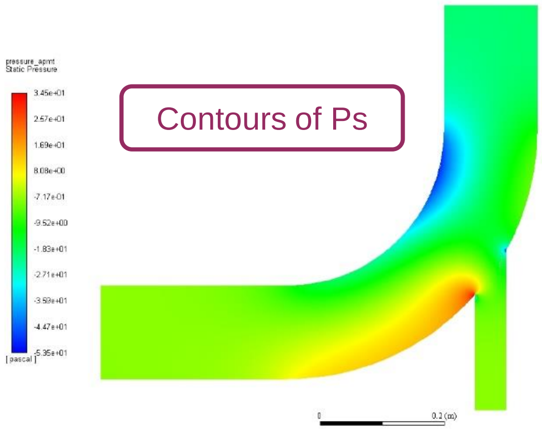
	C %	Si %	Mn %	Mo %	Cr %	Al %	Fe %
Nominal composition				3.0	21.0	5.0	Bal.
Min	-	-	-		20.5	-	
Max	0.08	0.7	0.4		23.5	-	

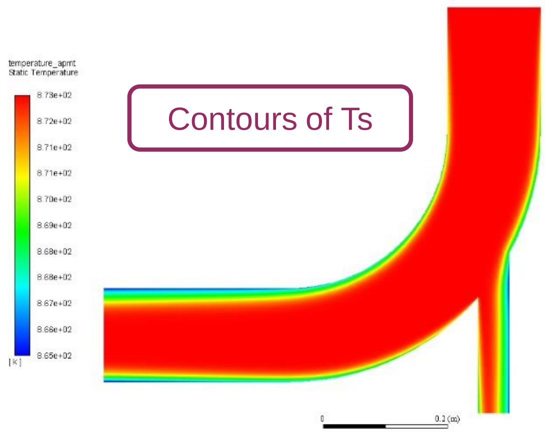
Temperature ºC	Thermal Expansión Coeff. x 10^{-6} / K
20 – 250	12.4
20 – 500	13.1
20 – 750	13.6
20 – 1000	14.7
20 – 1200	15.4

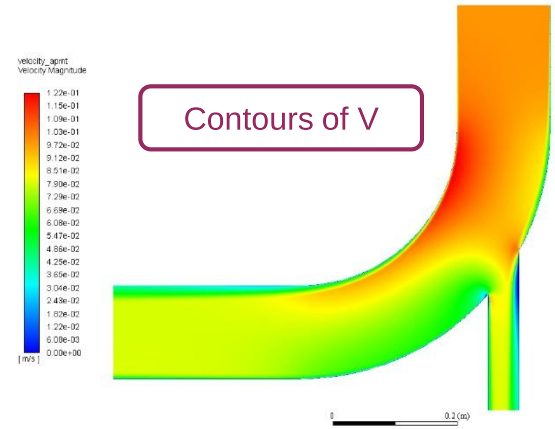
Density g/cm^3					7.25									
Electrical resistivity @ 20 ºC Ω mm^2/m					1.40									
Poisson's ratio					0.30									
T (ºC)	**20**	**100**	**200**	**300**	**400**	**500**	**600**	**700**	**800**	**900**	**1000**	**1100**	**1200**	**1300**
Young's modulus (GPa)	220	210	205	-	190	-	170	-	150	-	130	-	-	-
Temperature factor of resistivity (Ct)	-	1.00	1.00	1.01	1.01	1.01	1.02	1.02	1.02	1.03	1.03	1.03	1.03	1.04
Thermal conductivity (x 10^{-6}/K)	11	-	-	-	-	-	21	-	23	-	27	-	29	-
Specific heat capacity (kJ kg^{-1} K^{-1})	0.48	-	0.56	-	0.64	-	0.71	-	0.67	-	0.69	-	0.70	-
Melting point			1500 ºC											
Magnetic properties			The material is magnetic up to approximately 600 °C (Curie point)											
Emissivity - fully oxidized material			0.70											

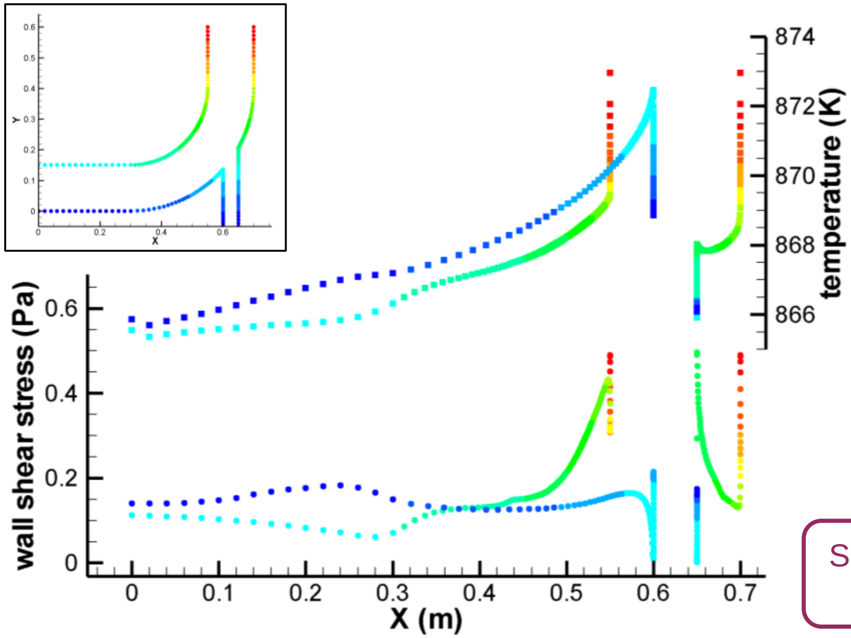
Data extracted from Kanthal datasheet and implemented in the solver

Preliminary CFD results – 2D steady & turbulent liquid-Pb flow









Parameters for CFD simulations	Values
Tube diameter (mm)	150
Inlet temperature (K)	873
Reynolds number (-)	10^5
Static Pressure (MPa)	0.1
Turbulence intensity (%)	5.0
Turbulent viscosity ratio (-)	5.0
Wall heat transfer coeff. ($W/m^2.K$)	20.0

Shear stress and wall temperature (coloured by the y-direction)

Following step:
CFD-FEM coupling to investigate the liquid-Pb coolant flow problem

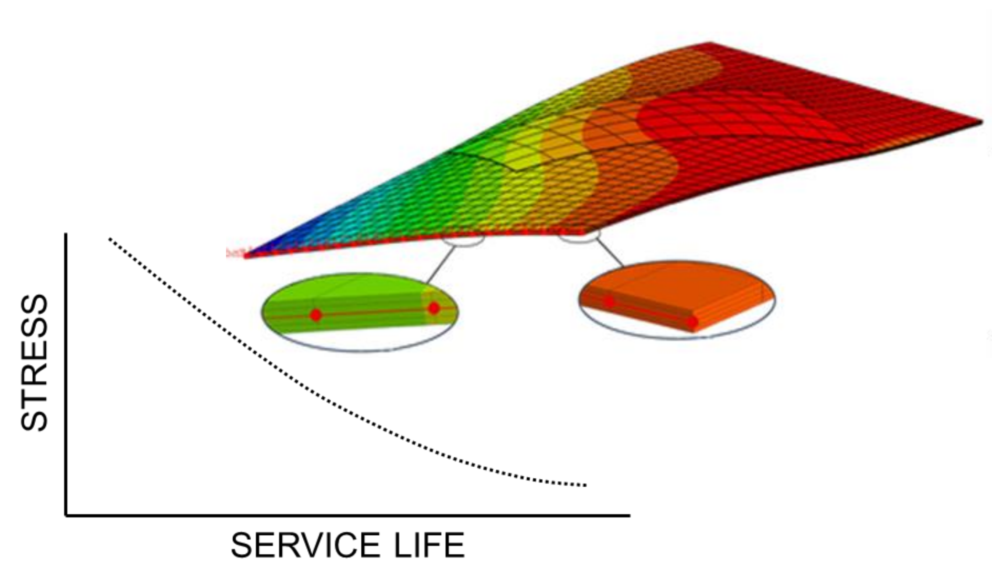
CFD solver ⟷ Coupled FEM

Hydrodynamic and thermal loading on the solid material extracted from CFD simulations

Structural study – thermal and stress analysis

GOALS:

- Investigate the variation of the mechanical properties of the Kanthal for real stress loading conditions
- Estimate with higher precision the service life of the Kanthal for liquid-Pb cooling nuclear applications



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