MATS9AI MATERIAL COMPUTATIONAL SIMULATION

MATS9AI Material computational simulation	Duration: 21 hours	ECTS Credits : 2	Semester : S9

Person(s) in charge :

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key words :

Prerequisites : Phase diagram and microstructures

Objective : Discover and manipulate major numerical tools to predict the microstructures and properties of materials (structural and functional applications)

Program and Contents :

This course aims at introducing the usefulness and the central role of numerical simulations for future “material” engineers. It covers actually the 4 main categories of material modeling (according to G. Martin’s classification):
• Modeling chemical link (first principle calculations)
• Modeling rapid events at atomic scale (molecular dynamics)
• Modeling slow aging kinetics and phenomena (phase transformations, phase diagrams)
• Link between microstructure and properties
In this field, being exhaustive is almost impossible. Students will thus be required to make individual literature survey on specific simulation techniques and softwares and present to their mates a summary of their findings (oral presentation). This S9 module permits to put into practice the scientific knowledge gained in S7-S8 in the frame of department courses and go deeper within certain fields. Students will be encouraged to use commercial and open-source softwares during tutorials.
Case studies (TD):
• Solidification of binary CuNi alloys (Calphad method and data mining)
• Simulation of TTT and CCT diagrams of special steels (Cambridge softwares suite)
• Prediction of the mechanical and thermal properties of Cermets (Quickfield)
• Practical use of Finite Elements commercial software (Abaqus)
• Ab initio DFT (Density Functional Theory) numerical simulations : application to Silicon
• Industrial tools for product line management

Abilities:

Levels	Description and operational verbs
Know	Discover the different classes of material modeling tools
Understand	Understand how numerical simulation works, the physical principles and the major calculation steps.
Apply	Mastering inputs and outputs of calculation software.
Analyse	Analyze the fidelity and accuracy of a numerical approach with respect to the experimental data
Summarise	Define the advantages and limits of the simulation technic (SWOT)
Assess	Evaluate the complexity and the relevance of a numerical approach with an material engineer background (Make or Buy strategy)

Evaluations :

☐ Written Test	☐ Continuous Control	☑ Oral Report	☐ Project	☑ Written Report