University of Puerto Rico
Mayagüez Campus
College of Engineering
Department of General Engineering
Master of Science and Engineering

Course Syllabus

1. General Information:

Alpha-numeric codification: CIIM 6015
Course Title: COMPUTATIONAL MATERIALS SCIENCE
Number of credits: 3
Contact Period: 2 hours of lecture and one two-hour laboratory per week

2. Course Description:

English: Study of the concepts of computer-assisted modeling and their applications to atomistic processes, which will permit the development of skills necessary for the computational analysis of processes such as kinetics and diffusion phenomena. The behaviors governed by isotropic or anisotropic properties (e.g., texture development) and phase transformation processes (e.g., segregation, precipitation, quenching), are also covered.

Spanish: Estudio de los conceptos de modelamiento asistido por computadora y su aplicación a procesos atomísticos que permitirá el desarrollo de destrezas necesarias para el análisis computacional de procesos tales como cinética y fenómenos de difusión. Los comportamientos gobernados por las propiedades isotrópicas o anisotrópicas tal como el desarrollo de texturas y procesos de transformación de fases tales como segregación, precipitación y templado son también cubiertos.

3. Pre/Co-requisites and other requirements:

4. Course Objectives:

By the end of the course students will:
- Describe the industrial need for process modeling.
- Identify the physical behaviors to be described for a given process, such as casting, forming and welding.
- Analyze the loads in idealized metal deforming operations (forging, wire drawing, rolling, extrusion, machining) using analytical plasticity (equilibrium equations and yield criteria, and upper bound methods).
- Analyze the heat flow and calculate temperature histories in idealized heat treatment, surface hardening of steels, and welding processes.
- Identify the important issues (material properties, boundary conditions, choice of mesh) in setting up a finite element model of a process.
- Apply knowledge of thermal and deformation history on the evolution of microstructure in materials and apply simple models of microstructure evolution in for example, phase transformation, grain growth and recrystallization.
- Identify the factors causing failure (microstructures, corrosion and residual stress).
- Evaluate the significance of processing as the origin of many component failures.

5. Instructional Strategies:

☒conference ☐discussion ☒computation ☐laboratory

☐seminar with formal presentation ☐seminar without formal presentation ☐workshop

☐art workshop ☐practice ☐trip ☐thesis ☒special problems ☐tutoring

☐research ☐other, please specify:

6. Minimum or Required Resources Available:

Computer laboratory S210

7. Course time frame and thematic outline

Outline	Contact Hours
- Process modeling and its industrial context.	3/0
- Analytical plastic analysis of forming processes, using equilibrium equations and yield criteria, and upper bound methods.	7/5
- Analytical heat flow analysis in heat treatment and welding.	8/5
- Introduction to numerical methods (finite element analysis) for thermo-mechanical process modeling.	7/9
- Modeling of micro-structure evolution during thermo-mechanical processing and subsequent properties.	3/5
- Processing as the origin of defects and failures (microstructure, damage, residual stress)	2/5
- Exam	1
Total hours: (equivalent to contact period)	30/30

8. Grading System

☒Quantifiable (letters) ☐ Not Quantifiable

Standard Curve:

100-90 A; 89-80 B; 79-70 C; 69-60 D; 59-0 F

9. Evaluation Strategies

	Quantity	Percent
☒ **Exams**	**1**	**25**
☒ **Final Exam**	**1**	**25**
☐ **Short Quizzes**		
☒ **Oral Reports**	**4**	**25**
☐ **Monographies**		
☐ **Portfolio**		
☒ **Projects**	**2**	**25**
☐ **Journals**		
☐ **Other, specify:**		
TOTAL:		**100%**

10. Bibliography:

Textbook:

Powers, M. T., Lavernia, E. J., Groza, J. R. & Shackelford, J.F. (Eds.). (2007). *Materials processing handbook*. Boca Raton, FL: CRC Press. http://dx.doi.org/10.1201/9781420004823 [Available via CRCNetBASE, UPRM General Library]

Other resources:

Advani, S. G., & Murat Sozer, E. (Eds.). (2002). *Process modeling in composites manufacturing*. http://dx.doi.org/10.1201/9780203910061 There is no newer version. [Available via CRCNetBASE, UPRM General Library]

Bao, W. (2012). *Multiscale modeling and analysis for materials simulation*. Hackensack, NJ: World Scientific. [Available at the Circulation Collection (TA342 .M84 2012), UPRM General Library]

Dixit, P. M., & Dixit, U. S. (Eds.). (2002). *Modeling of metal forming and machining processes: By finite element and soft computing methods*. http://dx.doi.org/10.1007/978-1-84800-189-3 There is no newer version. [Available via Springer eBooks, UPRM General Library]

Selected articles from: *Materials and Manufacturing Processes*. Taylor & Francis [Available online via EBSCO Business Source Complete, UPRM General Library]

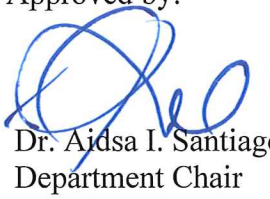
11. Academic Integrity: —The University of Puerto Rico promotes the highest standards of academic and scientific integrity. Article 6.2 of the UPR Students General Bylaws (Board of Trustees Certification 13, 2009-2010) states that academic dishonesty includes, but is not limited to: fraudulent actions; obtaining grades or academic degrees by false or fraudulent simulations; copying the whole or part of the academic work of another person; plagiarizing totally or partially the work of another person; copying all or part of another person answers to the questions of an oral or written exam by taking or getting someone else to take the exam on his/her behalf; as well as enabling and facilitating another person to perform the aforementioned behavior. Any of these behaviors will be subject to disciplinary action in accordance with the disciplinary procedure laid down in the UPR Students General Bylaws.—

12. According to Law 51: Students will identify themselves with the Institution and the instructor of the course for purposes of assessment (exams) accommodations. For more information please call the Student with Disabilities Office which is part of the Dean of Students Office at (787) 265-3864 or (787) 832-4040 extensions 2040 or 3372.

Prepared by:

Dr. Marcelo Suárez
Coordinator

Approved by:



Dr. Aidsa I. Santiago Román
Department Chair

Revised: June 2016