Advanced materials modeling

Basic information

Field of study Materials Science	**Didactic cycle** 2021/2022
Speciality All	**Subject code** CIMA00S.II2S.8b168f8a83532b6ca469a571408e68f2.21
Department Faculty of Materials Science and Ceramics	**Lecture languages** English
Study level Second-cycle studies	**Mandatory** Elective
Study form Full-time studies	**Block** Major Modules
Education profile General academic	**Subject related to scientific research** Yes

Subject coordinator	Robert Filipek
Lecturer	Robert Filipek, Krzysztof Szyszkiewicz-Warzecha

Period Semester 2	**Examination** Exam **Activities and hours** Lecture: 15, Seminars: 15	**Number of ECTS points** 2.0

Subject learning outcomes

Code	Outcomes in terms of	Directional learning outcomes	Examination methods
Knowledge – Student knows and understands:			
W1	Has extended knowledge in the field of higher mathematics, including: ordinary and partial differential equations, existence and uniqueness of initial, boundary and initial-boundary problems, optimization problems and methods of solving them.	IMT2A_W01	Activity during classes, Execution of a project, Test, Examination, Scientific paper

W2	Has knowledge on computer programming techniques and tools with the use of parallel programming, the use of multiprocessor machines, computing clusters and other advanced computing techniques. Has extended knowledge of computational methods and IT tools necessary for materials design and processes modeling.	IMT2A_W02	Activity during classes, Execution of a project, Test, Examination, Scientific paper
Skills – Student can:			
U1	He can communicate in the language of mathematics with specialists in various fields, including industry.	IMT2A_U04	Activity during classes, Execution of a project, Test, Examination, Scientific paper, Involvement in teamwork
Social competences – Student is ready to:			
K1	Understands the importance of the influence of materials engineering on the development of modern technologies. He understands the need for training and improving his professional and social competences	IMT2A_K01, IMT2A_K03	Activity during classes, Test, Examination, Scientific paper

Programme content that ensure achieving learning outcomes for the module

Basic knowledge of phenomenological modeling and numerical methods. Formulations and solutions of selected inverse problems. The use of COMSOL Multiphysics software and programming in C / C ++ and VBA to solve selected problems of mass, energy and momentum transport in 1D, 2D and 3D geometry.

Calculation of ECTS points

Activity form	**Average amount of hours* needed to complete each activity form**
Lecture	15
Seminars	15
Preparation for classes	10
Realization of independently performed tasks	8
Examination or Final test	2
Contact hours	5
Preparation of project, presentation, essay, report	5
Student workload	**Hours** 60
Workload involving teacher	**Hours** 30

* hour means 45 minutes

Study content

No.	Course content	Subject learning outcomes	Activities
1.	Selected ordinary and partial differential equations used in materials engineering. Examples of stationary and evolutionary problems in the area of: fluid dynamics diffusion in solid state chemical kinetics galvanostatic pulse methods electrochemical impedance spectroscopy Numerical methods of solving boundary and initial-boundary problems using finite differences, finite elements and finite volumes methods. Software used for numerical calculations. Inverse problems in materials engineering and njumerical methods and software for solving them. Examples of the use of inverse methods to determine the parameters of mathematical models.	W1, W2, U1, K1	Lecture
2.	Formulation and solution of selected models in the field of materials engineering, including: • model of the ions transport in the lithium-ion battery charging process • modeling of reinforcing bars corrosion in reinforced concrete materials • optimization of the heat transport process in the accumulation stove • modeling of transport processes in porous materials • the use of neural networks in optimization problems • ion transport in cell membranes • design and manufacture of gradient materials The use of various tools such as programming in VBA and C / C ++, Matlab and COMSOL Multiphysics software in materials engineering.	W1, W2, U1, K1	Seminars

Course advanced

Teaching methods:

Lectures, Multimedia presentation, Discussion, Project assignments, Blackboard exercises

Activities	Examination methods	Credit conditions
Lecture	Activity during classes, Examination	Exam
Seminar classes	Activity during classes, Execution of a project, Test, Examination, Scientific paper, Involvement in teamwork	Written test

Requirements and method of completing particular forms of classes

The necessary conditions for completing the course include:
1. attendance at at least 75% of lectures
2. Obtaining a grade of at least 3.0 from the exam
3. Obtaining a grade of at least 3.0 from the seminar

Method of calculating the final grade

The basis for the evaluation of the course is the arithmetic mean of the marks for the exam and the seminar with the following weights: 0.6 and 0.4.

Method and procedure for compensating for missed coursework resulting from student absence from classes

The student must make up for absences from classes (maximum 2 classes). The way of doing homework is agreed individually with the teacher.

Entry requirements

Basic skills in Visual Basic for Applications programing.

Attendance requirements for particular classes, with indication whether student attendance is compulsory

Lecture: Students participate in the classes, learning set by step the next teaching content in accordance with the syllabus of the course. Students should ask questions and explain doubts on a regular basis. Audio-visual recording of the lecture requires the consent of the lecturer.
Seminar classes: Students present the topic indicated by the teacher on the forum of the group and participate in the discussion on this topic. Both the substantive value of the presentation and the so-called soft skills are evaluated.

Literature

Obligatory

1. M. Rappaz, M. Bellet, M. Deville, Numerical Modeling In Materials Science and Engineering, Springer-Verlag Berlin Heidelberg 2003
2. R. Filipek, Modeling and inverse methods in materials engineering, Wydawnictwo Naukowe AKAPIT, Kraków, 2019.

Optional

1. R.L. Burden, J.D. Faires, Numerical Analysis third edition, Prindle, Weber & Schmidt, Boston 1988.
2. A. Quarterioni, Numerical Models for Differential Problems, Springer 2009.
3. M.E. Glicksman, Diffusion in Solids, JohnWiley & Sons 2000.
4. D. Britz, Digital Simulation in Electrochemistry, Springer, 3rd Ed. 2005.
5. E.B. Tadmor, R.E. Miller, R.S. Elliott, MContinuum Mechanics and Thermodynamics: From Fundamental Concepts to Governing Equations, Cambridge University Press 2012.
6. H.P. Langtangen, Computational Partial Differential Equations, Springer; 2nd Ed. 2003.
7. P. Šolin, Partial Differential Equations and Finite Element Method, Wiley-Interscience, 2006.
8. P. A. Nikrityuk, Computational Thermo-Fluid Dynamics, in Materials Science and Engineering,Wiley-VCH 2011.

Research and publications

Publications

1. 1. R. Filipek, “Interdiffusion in Multi-Component Systems Showing Variable Intrinsic Diffusivities”, Solid State Phenomena, 72, (2000), 165-170.
2. 2. B. Bożek, R. Filipek, K. Holly, C.Mączka, “Distribution of Temperature in Three-Dimmensional Solids”, Opuscula Mathematica, 20, (2000) 27-40.
3. 3. J. Nowacki, M. Danielewski, R. Filipek, “Brazed joints evaluation and computer modelling of mass transport in multi-component systems in the AuNi solder-14-5 PH joints”, J. Mat. Proc. Techn., 157-158, (2004), 213-220.
4. 4. J.J. Jasielec, R. Filipek, K. Szyszkiewicz, J. Fausek, M. Danielewski, A. Lewenstam, „Computer simulations of

electrodiffusion problems based on Nernst-Planck and Poisson equations”, Computational Materials Science, 63, (2012),75–90.

5. 5. A. Wierzbicka-Miernik, K. Miernik, J. Wojewoda-Budka, K. Szyszkiewicz, R. Filipek, L. Litynska-Dobrzyńska, A. Kodentsov, P. Zięba, „Growth kinetics of the intermetallic phase in diffusion-soldered Cu-5 at.%Ni/Sn/Cu-5 at.%Ni interconnections, Materials Chemistry and Physics, 142 (2–3), (2013), 682–685.
6. 6. K. Szyszkiewicz, J. J. Jasielec, M. Danielewski, A. Lewenstam, R. Filipek, “Modeling of Electrodiffusion Processes from Nano to Macro Scale”, Journal of The Electrochemical Society, 164 (11), (2017), E3559–E3568.
7. 7. R. Filipek, Modeling and inverse methods in materials engineering, Wydawnictwo Naukowe AKAPIT, Kraków, 2019.

Directional learning outcomes

Code	Content
IMT2A_K01	Rozumie potrzebę dokształcania się oraz podnoszenia swoich kompetencji zawodowych i społecznych oraz potrafi w sposób zrozumiały przekazywać informacje i krytyczne opinie dotyczące inżynierii materiałowej
IMT2A_K03	Ma świadomość ważności i zrozumienia pozatechnicznych aspektów i skutków działalności inżynierskiej, w tym jej wpływu na środowisko i związanej z tym odpowiedzialności za podejmowane decyzje, przestrzega zasady etyki zawodowej oraz rozumie znaczenie wpływu inżynierii materiałowej na rozwój nowoczesnych technologii
IMT2A_U04	Potrafi optymalnie dobrać metody i narzędzia służące do rozwiązania zadań typowych dla inżynierii materiałowej uwzględniających kryteria doboru materiału i procesu wytwórczego
IMT2A_W01	Ma poszerzoną i pogłębioną wiedzę w zakresie nauk podstawowych niezbędną do zrozumienia zjawisk występujących przy wytwarzaniu, badaniu oraz eksploatacji materiałów inżynierskich
IMT2A_W02	Ma poszerzoną wiedzę w zakresie metod obliczeniowych i narzędzi informatycznych niezbędnych do analizy wyników eksperymentów oraz projektowania materiałów i modelowania procesów.