FSH3141 Multi-scale Modeling of Nuclear Materials 6.0 credits

Flerskalemodellering av kärntekniska material

This is a translation of the Swedish, legally binding, course syllabus.

Establishment

Course syllabus for FSH3141 valid from Spring 2019

Grading scale

P, F

Education cycle

Third cycle

Specific prerequisites

The students should have an MSc in the field of physics or materials science.

Knowledge about the crystallographic structure of materials is needed for this class. A good material physics comprehension is also of great help.

Knowledge of principles such as diffusion, phase diagrams and electronic structure is also useful.

Language of instruction

The language of instruction is specified in the course offering information in the course catalogue.

Intended learning outcomes

The current and future nuclear industries are significantly impacted by the evolution of materials under irradiation conditions. Irradiation effects such as swelling, embrittlement and creep place strong limits on the lifetime of the structural materials and other components. With the development of the fourth generation nuclear reactor systems and nuclear fusion, the problems are amplified due to the strong presence of fast neutrons. Experiments on nuclear materials are expensive and time consuming, thus making reliable simulations and modeling an important part of the solution.

After this course, the students should be able to

1. describe, and when pertinent compare, different simulation techniques. The students should also be able to create a scheme using several of these techniques to cover a wider range in time and space.
2. apply each of the simulation techniques presented in the class for basic cases, using the computer codes provided. Additionally, they should be able to solve more complex problems using their previous knowledge in materials theory.
3. explain the limitations of the techniques and to select the one which is the most adapted to a specific problem. The students should be able to analyze their results and explain how they could be improved. They should know where to look for information about advanced simulation methods that will not be covered in this class.
4. present their results in the form of a presentation during a seminar and in the form of a report. They should be able to distinguish the most important points to present orally while giving more details in the written report. A clear scientific organization is expected for both media.

Course contents

The students will use the theoretical and practical background given in leactures and computer exercises in order to solve an original problem in the form of a project.

The teacher-led parts of the course consist of 7 lectures and 4 computer labs. The lectures are intended to last two hours.

1. Stakes and current possibilities of materials modeling

2. Damage mechanisms and influence of radiation

3. Density Functional Theory

4. Molecular dynamics and interatomic potentials

5. Kinetic Monte-Carlo and Rate theory – part 1

6. Kinetic Monte-Carlo and Rate theory – part 2

7. Linking techniques and introduction to further methods and techniques of interest

Each lab exercise is intended to take four hours. The students can choose, with the aid of the teacher, a

system they wish to model, provided that the needed resources are available.

1. Computer lab 1: application of Density Functional Theory

2. Computer lab 2: application of Molecular Dynamics

3. Computer lab 3: application of the Kinetic Monte-Carlo method

4. Computer lab 4: application of Rate Theory

Disposition

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1. Stakes and current possibilities of materials modeling
2. Damage mechanisms and influence of radiation
3. Density Functional Theory
4. Molecular dynamics and interatomic potentials
5. Kinetic Monte-Carlo and Rate theory – part 1
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2. Computer lab 2: application of Molecular Dynamics
3. Computer lab 3: application of the Kinetic Monte-Carlo method
4. Computer lab 4: application of Rate Theory

Course literature

Distributed by the teacher.

Examination

- SEM1 - Seminars, 1.5 credits, grading scale: P, F
- PRO1 - Project, 4.5 credits, grading scale: P, F

Based on recommendation from KTH's coordinator for disabilities, the examiner will decide how to adapt an examination for students with documented disability.

The examiner may apply another examination format when re-examining individual students.

If the course is discontinued, students may request to be examined during the following two academic years.

Other requirements for final grade

To pass this course, attendance is required. Absence should be notified beforehand and will result in extra tasks to fulfill.

The students will have to solve an original problem of their choosing using the tools that they have learned. The project will carry a real physical significance and not only be a textbook case. The project will require the combination of several of the techniques in a way that is typical of material research.

The results will be presented during a seminar and in a report. The students may work individually or in pairs.

Ethical approach

- All members of a group are responsible for the group's work.
- In any assessment, every student shall honestly disclose any help received and sources used.
- In an oral assessment, every student shall be able to present and answer questions about the entire assignment and solution.