Course Syllabus

Skoltech

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Course Title (in English)	Thermodynamics of Materials
Course Title (in Russian)	Термодинамика материалов
Lead Instructor	Kvashnin, Aleksandr

Here's a structure of the form below:

1. Annotation

Course Description

The course provides a graduate level overview of selected topics of materials science related to formation of material and its stability. We will begin with the stability of materials by defining the energy contributions responsible for the stability including configuration, vibrational, and thermodynamic contributions to Gibbs free energy. Next, we will consider phase transitions and phase diagrams of materials with various dimensionality. One of the important factors responsible for stabilization is the formation of defects. Types of defects in bulk and 2D materials will be discussed. Considering all the above we will move to discussion of properties of surfaces and thin films which are the most important materials for sensing, energy storage, catalysis, and other applications.

Аннотация

Курс предоставляет собой обзор отдельных тем материаловедения, связанных с образованием материалов и их стабильностью. Курс начинается с изучения стабильности материалов, определяя энергетические вклады, ответственные за стабильность, включая конфигурационный, колебательный и термодинамический вклады в свободную энергию Гиббса. Затем переходим к рассмотрению фазовых переходов и фазовых диаграмм материалов с различной размерностью. Одним из важных факторов, влияющих на стабильность материалов, является образование дефектов. В курсе будут рассмотрены типы дефектов в кристаллических и двумерных материалах. Учитывая все вышесказанное, мы перейдем к обсуждению свойств поверхностей и тонких пленок, которые являются важными материалами для зондирования, хранения энергии, катализа и других приложений.

2. Basic Information

Course Academic Level MSc PhD

Course Academic Level Master-level course suitable for PhD students

Number of ECTS credits 6

Course Prerequisites / Recommendations

The course relies on basic knowledge of theoretical physics, chemistry, condensed matter physics at undergraduate level. Ideally it should follow an introductory course in Materials Science and Introduction to Solid State Physics.

Type of Assessment Graded

Grading Scale

A: 86

B: 76

C: 66

D: 56

E: 46

Course Term (in context of Academic Year) Term 1

Students of Which Programs do You Recommend to Consider this Course as an Elective?

BSc Programs: , Masters Programs: Advanced Computational Science
Advanced Manufacturing Technologies
Applied Computational Mechanics
Materials Science, PhD Programs: Materials Science and Engineering

Maximum Number of Students

	Maximum Number of Students
Overall:	12
Per Group (for seminars and labs):	

Course Stream Science, Technology and Engineering (STE)

3. Course Content

ECTS Credit System – Reference Tool

Topic: Stability of solids, Summary of Topic: Thermodynamical, mechanical, dynamical stability , Contact Hours: Lectures: 4, Contact Hours: Seminars: 2, Contact Hours: Labs: 0, Non-contact

Hours: Student's Independent Study: 8
Topic: Gibbs free energy, Summary of Topic: Lattice dynamics, vibrational entropy, dynamical stability , Contact Hours: Lectures: 2, Contact Hours: Seminars: 4, Contact Hours: Labs: 2, Non-contact Hours: Student's Independent Study: 8
Topic: Configurational entropy, Summary of Topic: Mixing enthalpy, high-entropy materials (HEM), entropy in HEMs, examples, AI for prediction of HEMs , Contact Hours: Lectures: 2, Contact Hours: Seminars: 4, Contact Hours: Labs: 0, Non-contact Hours: Student's Independent Study: 12
Topic: Thermodynamics vs. kinetics, Summary of Topic: Metastable phases, transition state, reaction rate, energy barriers, role of temperature , Contact Hours: Lectures: 2, Contact Hours: Seminars: 0, Contact Hours: Labs: 2, Non-contact Hours: Student's Independent Study: 14
Topic: Phase transitions, Summary of Topic: Melting, solid-solid, how to predict phase transition from DFT, role of diffusion, nucleation, Contact Hours: Lectures: 2, Contact Hours: Seminars: 2, Contact Hours: Labs: 0, Non-contact Hours: Student's Independent Study: 8
Topic: Phase diagrams, Summary of Topic: Convex hulls, (P,T) phase diagrams, composition-energy, chemical potential-composition, diagrams for low-D systems, simulations, example, Contact Hours: Lectures: 2, Contact Hours: Seminars: 2, Contact Hours: Labs: 2, Non-contact Hours: Student's Independent Study: 8
Topic: Defects in solids, Summary of Topic: Points defects, interstitials, complexes, energy of formation, dislocations, grain boundaries, inclusions. Influence to mechanical properties, electronics, magnetism, defects in 2D materials, Contact Hours: Lectures: 2, Contact Hours: Seminars: 4, Contact Hours: Labs: 2, Non-contact Hours: Student's Independent Study: 8
Topic: Free surfaces of the crystals, Summary of Topic: Atomic structure, reconstructions, surface energy, electronic properties. Role of surface in catalysis, Contact Hours: Lectures: 4, Contact Hours: Seminars: 2, Contact Hours: Labs: 2, Non-contact Hours: Student's Independent Study: 10
Topic: Interfaces between materials , Summary of Topic: Structure and energetics, interfaces in solar cells (recombination, p-n transition), interfaces in batteries, charge transfer, diffusion, Contact Hours: Lectures: 2, Contact Hours: Seminars: 2, Contact Hours: Labs: 2, Non-contact Hours: Student's Independent Study: 12
Topic: Thin films, Summary of Topic: Role of substrates, stability of thin films, methods of synthesis, carbon films, non-carbon films, epitaxial growth, dependence on thickness, Contact Hours: Lectures: 4, Contact Hours: Seminars: 2, Contact Hours: Labs: 2, Non-contact Hours: Student's Independent Study: 10

4. Learning Outcomes

Please specify course intended learning outcomes using Skoltech Learning Outcomes Framework.

Skoltech Learning Outcomes are indicated as per Skoltech Learning Outcomes Framework.

1. FUNDAMENTAL KNOWLEDGE

1.1. KNOWLEDGE OF MATHEMATICS AND NATURAL SCIENCES

2. PERSONAL AND GENERAL PROFESSIONAL SKILLS AND ATTRIBUTES:

2.1. COGNITION AND MODES OF REASONING

2.1.1. Analytical reasoning and problem solving

2.1.4. Decision making (with ambiguity

urgency etc.)

2.2. ATTITUDES AND LEARNING PROCESS

2.2.3. Responsibility

intensity

perseverance

urgency and will to deliver

3. INTERPERSONAL SKILLS

3.1. COMMUNICATIONS IN INTERNATIONAL ENVIRONMENTS

- 3.1.1. Communications strategy and structure
- 3.1.2. Written
- electronic and graphical communication
- 3.1.3. Oral presentation and discussion

4. LEADING THE INNOVATION PROCESS

4.2. VISIONING — INVENTING NEW TECHNOLOGIES THROUGH RESEARCH

- 4.2.1. The research process — hypothesis
- evidence and defense
- 4.2.2. Basic research leading to new scientific discovery

4.3. VISIONING — CONCEIVING AND DESIGNING SUSTAINABLE SYSTEMS

- 4.3.4. Disciplinary and multidisciplinary design for sustainability
- safety
- aesthetics
- operability and other objectives

4.5. DELIVERING ON THE VISION — ENTREPRENEURSHIP AND ENTERPRISE

- 4.5.1. New venture conceptualization and creation

5. Assignments and Grading

In-person Attendance Requirement 80

Assignment Type: Computer Labs, Assignment Summary: Student successfully finished all tasks in the Lab, % of Final Course Grade: 20
Assignment Type: Final Project, Assignment Summary: Final project is the presentation according to the topic which student defines at the beginning of the course. Information from lectures and computer labs should help for preparation of the final project presentation., % of Final Course Grade: 30
Assignment Type: Class participation, Assignment Summary: Active participation in seminars, asking questions throughout the course, and answering the questions. , % of Final Course Grade: 50

6. Assessment Criteria

Select Assignment 1 Type

- Computer Labs

Sample Assigment 1:

Input Sample of Assignment 1 or Share a Link to Assignment 1

Relax the crystal structure given by lecturer using DFT code

Create slab with surface of specific direction
Calculate the surface energy of different slabs
Make a Wulff construction of the crystal

Assessment Criteria for Assignment 1

Obtain your own results according to your task, perform comparison with published experimental and theoretical data, if possible. Results should be presented as 1-2 page report or 5-min presentation of everything that you consider nontrivial in your work.

Input example in the text box or upload a file, for the next assignment to appear.

Select Assignment 2 Type

Final Project

Sample of Assigment 2:

Input Sample of Assignment 2 or Share a Link to Assignment 2

The final project can be related to your current or future research or can be given by instructor or supervisor.

It should be presented as conference-style presentation: 20-min, 15-30 slides including Introduction, Methods, Results, and Conclusion sections
Article-style report: 5-10 pages of original text + unlimited number of figures and tables + at least 10-20 references

Assessment Criteria for Assignment 2

Well prepared presentation about your project where you will discuss the results, methods that you used, and discussion why your result is similar to reference ones or not, explain possible explanation of that.

Select Assignment 3 Type

Class participation

Sample of Assigment 3:

Input Sample of Assignment 3 or Share a Link to Assignment 3

Active participation in seminars, asking questions throughout the course, and answering questions.
Discussing your course project during the course and at any other convenient time.
You should enjoy to learn new things

Assessment Criteria for Assignment 3

Participation in at least 80% of all classes of the cource. 100% of computer labs should be participated

Sample of Assigment 4:

Sample of Assigment 5:

Sample of Assigment 6:

Sample of Assigment 7:

Sample of Assigment 8:

Sample of Assigment 9:

7. Textbooks and Internet Resources

You can request at most two required textbooks. Additionaly, you can suggest up to nine recommended textbooks.

Required Textbooks: Neil W. Ashcroft, N. David Mermin, Solid State Physics , ISBN-13 (or ISBN-10): 978-0030839931

Recommended Textbooks: Richard J. D. Tilley , Defects in Solids , ISBN-13 (or ISBN-10): 978-0470077948
Recommended Textbooks: Harald Ibach, Physics of Surfaces and Interfaces, ISBN-13 (or ISBN-10): 978-3-540-34710-1

8. Facilities

Software: Quantum Espresso, python

Equipment: Room equipped with audio, video, WiFi

9. Additional Notes

Is this syllabus complete?	Yes, the syllabus is a final draft waiting for approval by Education Department
The proposed course 1) has explicit academic content and requirements for receiving credits, 2) is in alignment with the program's learning outcomes, 3) adheres to policies and Skoltech regulations.	Lead Instructor confirms
Syllabus status	Approved by the Education Department