Министерство науки и высшего образования Российской Федерации
НАЦИОНАЛЬНЫЙ ИССЛЕДОВАТЕЛЬСКИЙ
ТОМСКИЙ ГОСУДАРСТВЕННЫЙ УНИВЕРСИТЕТ (НИ ТГУ)

Механико-математический факультет

УТВЕРЖДАЮ:
Декан ММФ ТГУ

Л. В. Гензе

Оценочные материалы дисциплины

Математическое моделирование наноструктурных материалов

по направлению подготовки

01.04.01 Математика

Направленность (профиль) подготовки :
Математический анализ и моделирование (Mathematical Analysis and Modelling)

Форма обучения
Очная

Квалификация
Магистр

Год приема
2023

СОГЛАСОВАНО:
Руководитель ОП
А.В. Старченко

Председатель УМК
Е.А. Тарасов

Томск – 2023

MINISTRY OF SCIENCE AND HIGHER EDUCATION
OF THE RUSSIAN FEDERATION
NATIONAL RESEARCH TOMSK STATE UNIVERSITY

FACULTY OF MECHANICS AND MATHEMATICS

APPROVE:
Dean of FMM
Genze L.V.

Assessment materials for the discipline

Nanostructures material modeling

Field of study

Mathematics – 01.04.01

Master's degree program:
Mathematical analysis and modeling

Form of study
Intramural

Qualification
Master

Year of admission
2023

APPROVE:
Head of the program
Starchenko A.V.

Chairman of the E&MC
Tarasov E.A.

Tomsk – 2023

1. Competencies and indicators of their achievement, verified by these assessment materials

The goal of mastering the discipline is to develop the following competencies:

PC-1 Able to independently solve research problems within the framework of the implementation of a scientific (scientific, technical, innovative) project.

The results of mastering the discipline are the following indicators of achievement of competencies:

IPC–1.1 Conducts research aimed at solving individual research problems

IPC–1.2 Defines methods for the practical use of scientific (scientific and technical) results

IPC–1.3 Provides mentoring during the research process.

2. Assessment materials of current control and assessment criteria

Elements of current control:

– tests;

– colloquia.

Test (IPC–1.1)

Examples of test questions:

1. The density of the distribution function of the value x is described as $f(x) = Ae^{-U(x)/kT}$. This is the distribution::
   a) Gibbs
   b) Boltzmann
   c) Maxwell
   d) Gaussian
2. The ergodic hypothesis states that:
   a) the probability of a particle being in the j-th cell, determined by the formula $\widetilde{P_j} = \lim_{T\to\infty} T_j/T$ is not equal to the probability $P_j = \frac{N_{aj}}{N_a}$
   b) the average value of an observed physical quantity taken over the system under consideration is equal to the average value taken over time
   c) for any system in the ensemble, its relative time of stay in each of the microstates is not equal to the relative number of systems in the ensemble located in this microstate
   d) the time average of a system's properties is equal to the ensemble average of those properties.
3. In the equilibrium state of the phases of a two-phase system, the equality is satisfied
   a) phase pressures
   b) phase temperatures
   c) specific volumes of phases
   d) specific entropies of phases
   e) chemical potentials of phases
   f) internal phase energies

Keys: 1 b), 2 d), 3 a), b), e)

Evaluation criteria: the test is considered passed if the student answers at least half of the questions correctly.

Colloquia (IPC–1.2, IPC–1.3)

Examples of colloquia questions:

1. What are fluctuations of physical quantities

2. What is entropy
3. Formulate the meaning of the Maxwell distribution over the velocities of molecules
4. Formulate the first law of thermodynamics
5. Formulate the second law of thermodynamics
6. Formulate the third law of thermodynamics
7. Van der Waals forces
8. What is surface tension
9. What is an isobar
10. What is an isotherm
11. Kihara's Potential
12. Buckingham Potential
13. Morse potential
14. Peschl-Teller potential
15. Continuum model of nanostructure representation
16. Discrete model of nanostructure representation
17. Hybridization of electron shells
18. What are liquid membranes

Evaluation criteria: the colloquia is considered passed if the student answers at least half of the questions correctly.

3. Evaluation materials for final control (interim certification) and evaluation criteria

The examination ticket consists of two parts.

The first part contains two theoretical questions randomly selected by the student from the proposed list, testing IPC–1.1, IPC–1.2, IPC–1.3 Answers to the questions of the first part are given in detailed form after an hour of preparation without using recordings of lectures and practical classes or additional materials.

The second part contains up to 5 additional questions on the topics of lecture classes missed by the student, testing IPC–1.1, IPC–1.2, IPC–1.3. The answer to the question in the second part is given in a brief form without preparation.

List of theoretical questions:

1. Model of a material body. Aggregate states of matter. Basic signs of states of aggregation.
2. Ideal gas model. Methods for describing the behavior of particle systems.
3. Elementary probability theory. Classical and geometric definition of probability.
4. Macroscopic and microscopic conditions. Difference between microstates by positions and velocities.
5. Statistical ensemble of systems. Postulate of equiprobability.
6. Calculation of ensemble and time averages. Ergodic hypothesis.
7. Calculation of the probability of a macrostate.
8. Most probable number of particles.
9. Average number of particles per volume. Fluctuations. Relative magnitude of fluctuations.
10. Canonical ensemble. Gibbs distribution.
11. Density of states.
12. Maxwell distribution. Distribution density. Characteristic speeds.
13. Frequency of impacts of a molecule on a wall. Number of molecules in different parts of the Maxwell distribution. The principle of detailed balance.
14. Independence of probability densities of particle coordinates and velocities. Boltzmann distribution.
15. A mixture of gases in a vessel. The atmosphere of the planets.
16. Basic equation of the kinetic theory of gases. Clapeyron–Mendeleev equation.

17. Dalton's law. Lifting force.

18. Thermometric body and thermometric quantity. Thermometric temperature scale. Thermometers.

19. Third law of thermodynamics. Energy distribution over degrees of freedom.

20. Brownian motion. Problems of thermodynamics. Job.

21. Heat capacity. Heat capacity at constant volume and constant pressure. Relationships between heat capacities.

22. Types of polytropic processes. Process equations.

23. Entropy of an ideal gas. Physical meaning of entropy. Entropy change in an ideal gas.

24. Cycle work. Efficiency.

25. Carnot cycle. Second law of thermodynamics. Refrigerator and heater.

26. Bonding forces in molecules. Intermolecular forces in solids. Van der Waals forces. Potential of intermolecular interaction.

27. Deviation of gas properties from ideal. Virial equation of state. Van der Waals equation. Virial form of the van der Waals equation.

28. Isotherms of the van der Waals equation. Metastable states.

29. Critical parameters. Van der Waals law of corresponding states of gas.

30. Scheme of the Joule-Thomson experiment. Joule-Thomson effect.

31. Differential Joule – Thomson effect in real gas. Temperature difference in the process for van der Waals gas

32. Inversion temperature. Deviation of gas from ideality. Scheme of the Linde method.

33. Phase transformations. Two-phase liquid-vapor system. Clapeyron-Clausius equation.

34. Free energy of the surface. Thermodynamics of surface tension.

35. Kinematic characteristics of molecular motion: cross section, mean free path. Experimental determination of the collision cross section.

36. Cross section of collisions in the hard sphere model.

37. General transport equation. Transport equations for the stationary case: thermal conductivity, viscosity, diffusion.

38. Time-dependent transport equations.

39. Relaxation time for particle concentration. Transport phenomena in rarefied gases.

40. Transfer phenomena in solids.

41. Transfer phenomena in liquids.

Evaluation criteria:

The exam results are determined by grades “excellent”, “good”, “satisfactory”, “unsatisfactory”.

An “excellent” grade is given if the current control has been successfully passed (tests and all tasks for independent solution with a “pass” grade) and if detailed correct answers have been given to all theoretical questions of the first part and correct answers have been given to most of the additional questions. The student clearly, reasonably and logically presented his answers to the questions posed.

A “good” grade is given if the current control has not been completely passed (tests passed, but less than half of all tasks for independent solution with a “passed” grade) and if detailed correct answers are given to all theoretical questions of the first part or correct answers are given, but not everything is presented in detail and logically structured, and incorrect answers to most of the additional questions are given.

A “satisfactory” grade is given if the current control has not been fully passed (one of the tests has not been passed and less than half of all tasks for independent solution have been given with a “passed” grade) and if, in general, correct answers have been given to all the questions of the first part, but they are stated superficially and in violation of the logic of presentation and incorrect answers were given to most of the additional questions

An “unsatisfactory” grade is given if the current control has not been passed (tests have not been passed and less than half of all tasks are available for independent solution with a “pass” grade) and if the answers are presented very superficially and in violation of the logic of presentation; the student has very poor command of basic models and concepts; significant terminological and factual errors were made; incorrect answers were given, clearly a misunderstanding of the exam questions.

4. Assessment materials for testing residual knowledge (formation of competencies)

Test (IPC–1.1)

Examples of test questions:

1. The density of the distribution function of the value x is described as $f(x) = Ae^{-U(x)/kT}$. This is the distribution::
   a) Gibbs
   b) Boltzmann
   c) Maxwell
   d) Gaussian
2. The ergodic hypothesis states that:
   a) the probability of a particle being in the j-th cell, determined by the formula $\widetilde{P_j} = \lim_{T\to\infty} T_j/T$ is not equal to the probability $P_j = \frac{N_{aj}}{N_a}$
   b) the average value of an observed physical quantity taken over the system under consideration is equal to the average value taken over time
   c) for any system in the ensemble, its relative time of stay in each of the microstates is not equal to the relative number of systems in the ensemble located in this microstate
   d) the time average of a system's properties is equal to the ensemble average of those properties.
3. In the equilibrium state of the phases of a two-phase system, the equality is satisfied
   a) phase pressures
   b) phase temperatures
   c) specific volumes of phases
   d) specific entropies of phases
   e) chemical potentials of phases
   f) internal phase energies

Keys: 1 b), 2 d), 3 a), b), e)

Developer information

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