SUMMARY

Of the PhD Thesis on the Specialty «6D072300 – Technical Physics»

A.B. Bazarbek «Ab initio modeling of Fe-Ni-phosphides and Ni-sulfides at high-pressures with implication for composition and differentiation of planetary cores»

The aim of the dissertation research

The aim of this research is to determine the possible stable compounds and their structures in the Fe-P, Ni-P, Ni-S systems, as well as their phase relations at the pressures relevant to the Earth's core.

Research objectives

1. To perform crystal structure prediction calculations for stable phases in the Fe-P, Ni-P and Ni-S systems in the pressure range of 100–400 GPa.

2. To determine the stability fields for the found structures Fe_xP_y, Ni_xP_y and Ni_xS_y.

3. To calculate the phonon spectra and determine the dynamic stability of the predicted phases.

4. To perform spin-polarized calculations to determine the pressure of the disappearance of the magnetic moment.

5. To perform a structural analysis of the predicted phases.

Research methods

In this work, evolutionary algorithms implemented in the USPEX software package were used to search for intermediate compositions and crystal structures. The optimization and calculation of the electronic structure were carried out within the framework of the density functional theory using the plane wave basis, the PAW formalism and the generalized gradient approximation implemented in the VASP software package. The supercellular method and the finite shift method were used to calculate the phonon spectra. This calculation was also carried out within the framework of the density functional theory.

The main provisions (proven scientific hypotheses and other conclusions that are new knowledge) submitted for defense

1. The Fe-P system is characterized by two intermediate compounds Fe_2P and FeP at the pressure of the inner core of the Earth. The most iron-rich phosphide under these conditions is Fe_2P.

2. The Ni-P system is characterized by the presence of solid solutions and three intermediate compounds Ni_8P_3, Ni_2P and NiP_2 at pressures of 100–400 GPa.

3. The Ni-S system is characterized by the presence of solid solutions and three intermediate compounds Ni_3S, Ni_2S and NiS_3 at pressures of 100-400 GPa.

Description of the main results of the study

In the dissertation work, new structures in the Fe-P, Ni-P and Ni-S systems were predicted for the first time, their dynamic stability was established by calculating phonon spectra and the dependences of the magnetic moment on pressure for all the structures found were displayed. The stability fields of the found Fe_xP_y, Ni_xP_y and Ni_xS_y structures are determined, where it is indicated which stoichiometries are stable over the entire pressure range of 100–400 GPa and which stoichiometries break up into isochemical mixtures, being unstable at certain pressures. In addition, the dissertation shows intermediate compounds at the pressures of the the Earth's inner core.

Substantiation of the novelty and importance of the results obtained

In this dissertation, the phase relations in the Fe-P system up to 400 GPa are correctly determined. It should also be noted that in this work, for the first time, the Ni-P and Ni-S system was studied at the Earth's core pressures and the phase relations in these systems were established. The possible miscibility limits of S and P in the Ni structure at the Earth's core pressures were established.

The results obtained in the course of this study are of a fundamental nature and are important for further research of the structure and composition of the cores of the Earth and planets. Also, the data obtained will help determine priority areas for future research.

Compliance with the directions of scientific development or state programs

The dissertation work corresponds to the priority directions of science development that are being implemented in the Republic of Kazakhstan and contains new scientifically based theoretical results, the totality of which is important for the development of the studied scientific directions.

Description of the applicant's contribution to the preparation of each publication

All theoretical calculations of the dissertation research were carried out personally by the author with the participation of employees of the Laboratory of experimental Geochemistry and petrology of the Earth's Mantle of Novosibirsk State University and the laboratory of phase transformations and diagrams of the state of the Earth's matter under high pressures of the Sobolev Institute of Geology and Mineralogy of the Siberian Branch of the Russian Academy of Sciences. Processing and analysis of the results were carried out jointly with scientific consultants.

The main results of the dissertation research are published in printed works that fully correspond to the topic of the dissertation: 1 of them is an article in a peer-reviewed scientific journal included in the Web of Science and Scopus

database and related to the Q1 quartile in accordance with JCR Thomson Reuters, 4 articles in scientific publications recommended by committee on quality assurance in the field of science and education of the Ministry of education and science of the Republic of Kazakhstan, 10 theses and reports in the proceedings of international scientific conferences.