УДК 551.16 + 538.91

IRON PHOSPHIDES IN THE COMPOSITION OF THE EARTH'S CORE AND THE INFLUENCE OF MAGNETIC ORDER ON THE EQUATION OF STATE

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Abstract

This article discusses the role of iron phosphide in the composition and structure of the earth's core, which describes that nowadays, is well known that the Earth's inner core is dominantly composed of iron and a small fraction of nickel, with the presence of some light element. One of the likely candidate light element for the inner core is phosphorus. Because of the difficulties of experimental studies at high temperatures and pressures of the Earth's core, computer simulation using modern quantum chemical methods is of particular relevance. Also in this work, using quantum-chemical modeling from first principles within the framework of the density functional methods considered the influence of magnetic moment on the equation of state *P(V)* for two structures of iron phosphide Fe_3P at zero temperature and pressures up to 200 GPa. It is shown that the behavior of the function *P(V)* depends on the magnetic order and for each structure affects differently.

Keywords: Iron phosphide, Earth's core, first-principle calculations, quantum chemical modeling, magnetic moment.

ФОСФИДЫ ЖЕЛЕЗА В СОСТАВЕ ЯДРА ЗЕМЛИ И ВЛИЯНИЕ МАГНИТНОГО МОМЕНТА НА УРАВНЕНИЕ СОСТОЯНИЯ

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Аннотация

В данной статье рассматривается роль фосфида железа в составе и структуре ядра Земли, в которой описывается, что в настоящее время хорошо известно, что внутреннее ядро Земли состоит преимущественно из железа и небольшой доли никеля, с наличием некоторого легкого элемента. Одним из вероятных легких элементов для внутреннего ядра является фосфор. Учитывая трудности экспериментальных исследований при высоких температурах и давлении ядра Земли, компьютерное моделирование с использованием современных квантово-химических методов приобретает особую актуальность. Так же в данной работе с помощью квантово-химического моделирования из первых принципов в рамках метода функционала плотности рассмотрено влияние магнитного упорядочения на уравнение состояния *P(V)* для двух структур фосфида железа Fe_3P при нулевой температуре и давлении вплоть до 200ГПа. Показано, что поведение функции *P(V)* зависит от учета магнитного порядка и для каждой структуры влияет по-разному.

Ключевые слова: Фосфид железа, ядро Земли, первопринципные расчеты, квантово-химическое моделирование, магнитный момент.

Introduction

In recent years, the study of the composition of the Earth's core is still a relevant topic, which is essential for understanding the processes taking place on our planet. The processes of global differentiation and migration of matter in the earth's interior are associated with the problem, including the composition and structure of the nucleus. Of course, for many years, research has been carried out using high-precision geophysical measurements and various laboratory experiments at pressures and temperatures of the core and the lower mantle of the Earth. However, questions concerning the composition and structure of the core and lower mantle of the Earth remain far from unambiguous solutions and require even more attention and research using a large amount of isotope-geochemical and cosmochemical data.

The core of the Earth is the central and deepest part of our planet, located under the mantle of the Earth. The estimated depth of 2900 km, and reaches the Core is about 32 mass%, and 16% of Earth's volume and is responsible for the P–T parameters from 136 GPA and 3800-4200 K to 364 GPA and 5000-6000 K [1].

On the composition of the core, there are only indirect data obtained in different ways. Modern experiments with shock compression of metals and their compounds, as well as the data of static compression of these substances in heavy-duty diamond presses. Taking into account the data on the prevalence of chemical elements in the Solar system and on Earth, allow us to assume with a high degree of reliability that the Earth's core contains about 90% iron.

However, the outer core cannot consist only of pure iron and especially of its alloy with nickel, since the density of iron and nickel-iron of meteorite composition at pressures prevailing in the Earth's core is approximately 10–15% higher than the density of “nuclear” matter in the outer core Earth. It follows that, in addition to iron, a “nuclear” substance should contain light additives, which somewhat decrease the density of the substance. Among such additives is considered light elements like hydrogen, oxygen, carbon, sulfur, silicon and phosphorus [2].

Because of the difficulty of conducting experimental studies at temperature and pressure corresponding to the conditions of the Earth’s core, computer simulation using modern quantum-chemical methods of the iron phosphides as essential components of the Earth’s core is of particular relevance.

In this regard, it is necessary to note the calculations from first principles (Ab initio) for the study of the composition and differentiation of planetary nuclei. Modeling using ab initio methods helps to solve problems from the first fundamental principles without invoking additional empirical assumptions, that is, by directly solving the equations of quantum mechanics.

Research method

In this article, all calculations were carried out using quantum chemical modeling of the first principles in the framework of the density functional method - using the basis of plane waves. The simulation was carried out without taking into account the motion of atoms, that is, at zero temperature (T=0). Both spin-polarized and non-magnetic moment calculations were performed. The calculation parameters are as follows: the circumcision energy was 700 eV, the density of k-points was - 0.2 $Å^{-1}$. When modeling iron phosphide Fe_3P, two structures of different symmetry were chosen: *I-4* and *Cmcm*. Fe_3P-*I-4* - tetragonal symmetry, also known as schreibersite [3]. Fe_3P-*Cmcm* – recently found a new structure having rhombic polymorph [4].

Result of calculation

The results of the first-principle calculations of the equation of state for the structures Fe_3P-*Cmcm* and Fe_3P-*I-4* are shown in fig. 1-2. First of all, we constructed the equation of state *P(V)* for our two structures. A comparison of the *P(V)* dependence behavior for the magnetic and non-magnetic phases shows that for Fe_3P-*Cmcm* structure the behavior of the equation of state is exceptionally weakly dependent on taking into account the magnetic order in the system.

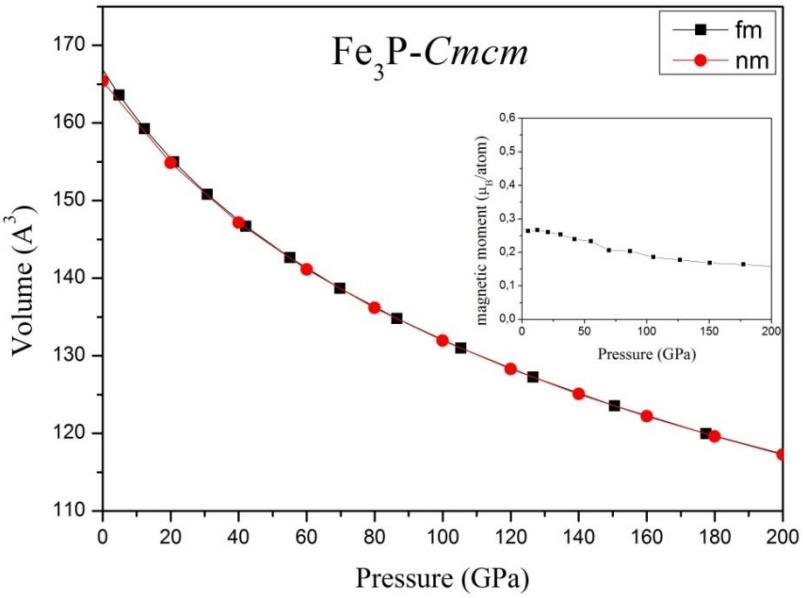

Figure 1. The dependence of the volume (with and without allowance for the magnetic moment) from the pressure for Fe_3P-*Cmcm*

At the same time, as can be seen from figure 2 for Fe_3P-*I-4* structure, the behavior of *P(V)* at relatively low pressures below 60 GPa is very different for the magnetic and non-magnetic phases. To explain this effect, the dependence of the magnetic moment on iron atoms as a function of pressure is additionally considered. For the Fe_3P-*I-4* structure at relatively low pressures, more precisely below 40 GPa, the magnetic moment on iron atoms is several times greater than the similar value for the Fe_3P-*Cmcm* structure. In this case, for the Fe_3P-*I-4* phase, there is a sharp decrease in the magnetic moment in the pressure range from 40 to 60 GPa, which coincides with the pressure range at which the differences in the behavior of the *P(V)* functions for the magnetic and non-magnetic phases disappear. At pressure from 60 GPa to 140 GPa, the value of the magnetic moment changes very little and amounts to approximately 0.4 μ_B on the iron atom. In the case of Fe_3P-*Cmcm* structure, the value of the magnetic moment in the entire range of the considered pressures varies in the range 0.2-0.3 μ_B and the account of the magnetic ordering has practically no effect on the behavior of the equations of state *P(V)*.

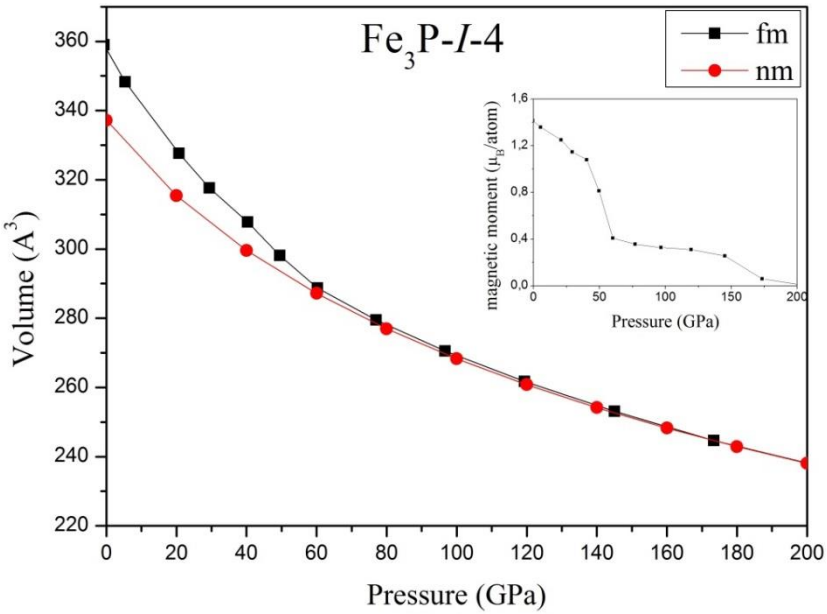

Figure 1. The dependence of the volume (with and without allowance for the magnetic moment) from the pressure for Fe_3P-*I-4*

Conclusions

The obtained results showed a strong influence of magnetic ordering on the behavior of the equation of state of iron phosphide Fe_3P *I-4* in the pressure range below 60 GPa, where the magnetic moment on iron atoms is significantly larger compared to the same value at higher pressures. For the Fe3P-*Cmcm* structure, the influence of the magnetic moment on the *P(V)* function is much weaker, which is associated with a much smaller magnitude of the magnetic moment in this phase and its weak dependence on pressure. In the future, it is planned to construct the equation of state *P(V)* depending on the temperature and phase stability diagrams of the various phases of the compounds in the *T-P* plane.

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