The Study on the Structure of Pure Iron Under A High Pressure of 100GPa

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Abstract: Using a new crystal structure prediction software CALYPSO (Crystal Structure Analysis by Particle Swarm Optimization), a new phase F222 of pure iron was obtained in a high pressure of 100GPa, which is different to δ-Fe, γ-Fe, α-Fe, the structure is a orthogonal structure, with this structure, the element Fe has the lattice parameters a=1.8459, b=10.6604, c=3.7637, α=β=γ=90°. The electric structures of the element Fe with F222 structure have also been studied, and the results of density of states revealed that the element Fe is a non-magnet.

Keywords: Structure, Pure Iron, Band Structure, CALYPSO, Phase

1. Introduction

The iron is a chemical element, its chemical symbol is Fe, atomic number is 26, is a transition metal, and its content in the crust is the second highest in the metal element content. Pure iron is white or silvery white, metallic luster, melting point 1538°C, and the boiling point 2750°C. Pure iron has good ductility, conductivity, thermal conductivity, and it is a magnetic material. The iron is an indispensable metal in the industrial sector, iron and a small amount of carbon can produce steel, which is not easy to demagnetize after magnetization, and it is a good hard magnetic materials. The iron is a more lively metal, in the metal activity sequence table, iron element is in front of hydrogen, iron chemical properties are more lively, and it is a good reducing agent. The iron can not burn in the air, but it can burn violently in the oxygen, it is a variable element, 0 price only has a reduction ability, +6 price only with oxidation ability, and with +2, +3 price, the iron has both reductive and oxidative ability. The iron element is also one of the essential elements of the human body. An adult body contains about 4 to 5 grams of iron, of which, 72% is in the form of hemoglobin, 3% in the form of myoglobin, 0.2% in the form of other compounds, and the rest is in the form of the reserve iron. There are three kinds of element Fe, namely δ-Fe, γ-Fe, α-Fe. In the temperature range of 1538°C to 1394°C, Fe crystallizes in a non-magnetic body-centered cubic lattice, the lattice parameter is a=0.293nm, named δ-Fe. In the temperature range of 912°C to 770°C, following a phase transition, δ- Fe changes into a non-magnetic face-centered cubic lattice, the lattice parameter is a=0.364nm, named γ-Fe. When the temperature is below 770°C, following another phase transition, the iron crystallizes into a magnetic body -centered cubic lattice (α-Fe), the lattice parameter is a=0.286nm [1-2]. Both the δ-Fe and α-Fe are body-centered cubic lattice, but the lattice parameters are not same, so the interactions between the atoms are different, so the physical and chemical properties are also diverse.

As we know, that the radius of the earth's internal mantle is about 2,900 km, the temperature is about 1500 ~ 3000°C, the pressure is of 500,000 to 1.5 million atmospheric pressure, the radius of the core is about 3500 km, the temperature is about 5540°C, and the pressure is about 3.5 million atmospheric pressure. In some earth-like planets, if the planets are far from the stars, the temperature is relatively low, so how does the iron element spread over on the planets under the millions of atmospheric pressure in the crust? At present, this research is still relatively small, in this paper, using a new crystal
structure prediction software CALYPSO (Crystal Structure Analysis by Particle Swarm Optimization), we studied the structure and magnetism of iron at 1 million atmospheric pressure.

CALYPSO is a short name of “Crystal Structure Analysis by Particle Swarm Optimization”, it has been developed by professor Ma and his team in Jilin university. It is designed to predict crystal structures of materials ranging from 0-dimensional (0D) to 1D, 2D, and 3D [3-10]. In the software, the Particle Swarm Optimization (PSO) algorithm is applied, and this algorithm is inspired by team organization pattern of a bird flock which can be regarded as a distributed algorithm in multidimensional searching and can be seen as an unbiased global optimization method [11]. The software can employed the structure relaxation software such as Vasp, Pwscf, Castep, Gaussian, etc. In the prediction of structures of a material, the CALYPSO can randomly generate a group structures of the material formula, for each structure, the geometry optimization will be make, the reasonable structures will be reserved and make further optimization, the unreasonable will be discarded, and this procedure will be repeat many times.

2. Computational Details

For pure iron, the number of element specie, name of the element Fe, the atom numbers, the number of formula, a estimate volume of the formula and the distance of the atoms were all supplied to the CALYPSO software, the maximum step of the revolution in the procedure was 30. The applied pressure was 100GPa, and the condition in one atmospheric pressure was also studied.

3. Results and Discussions

According the computational results, taking into account the experimental data, we obtained the three allotropes of element Fe, the structures are shown in figure 1.

The density of states (DOS) of the structure of α -Fe is obtained using a generalized-gradient approximation (GGA) method proposed in 1996 by Perdew, Burke and Emzerhof [12-15]. In the figure, one can see that the shapes of upper halves and the lower halves are asymmetry, especially around the Fermi level, there is a larger exchange splits, leading a large magnetic moment of 2.28µB of iron Fe.

![Figure 1. The three allotropes of element Fe. (a) δ-Fe, (b) γ-Fe, (c) α-Fe.](image)

![Figure 2. The calculated total DOS for the structure of α-Fe.](image)

![Figure 3. Majority spin band structures for α-Fe. The zero of energy denotes the position of the Fermi level.](image)

Using the CALYPSO software, the structure of element Fe under 100GPa pressure has been studied. The results reveal that the F222 crystal structure of element Fe is the most stable structure under 100GPa, as shown in the figure 4. The crystal positions described with the Wyckoff coordinates are 4c (0.25, 0.75, 0.75), 8f (0, 0.91, 0), and the lattice parameters are a=1.8459, b=10.6604, c=3.7637, α = β = γ
=90°. F222 is an orthogonal structure, which is obviously different to body-centered cubic and face-centered cubic lattice, element Fe with this structure should have different physical and chemical properties, so, we studied the electric structure of it.

The DOS of the structure F222 of Fe is obtained using a GGA method, as shown in the figure 5. In the figure, one can see that the electrons are compressed near the Fermi level compare to that of α-Fe, the shapes of upper halves and the lower halves are strictly symmetry, so, there is no exchange splits between the atoms, and the element is a non-ferromagnetic material, it is interesting, for δ-Fe and γ-Fe phase have no ferromagnetic property, now, there is a new phase F222 which is also not a magnet, and the ferromagnetic property is dominated not by temperature but by high pressure.

4. Conclusion

In summary, the structure of element Fe under a high pressure was studied in the paper using a new crystal structure prediction software CALYPSO, it was found that the F222 structure has the lowest energy in the high pressure of 100GPa (1 million atmospheric pressure), and the structure is different to the three known isotopes of element Fe (δ-Fe, γ-Fe, α-Fe), and with this structure, element Fe has no ferromagnetic property.

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References


