Advances in Materials
2017; 6(2): 7-10
http://www.sciencepublishinggroup.com/j/am
doi: 10.11648/j.am.20170602.11
ISSN: 2327-2503 (Print); ISSN: 2327-252X (Online)

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

Lei Feng[1, 2, *], Fei Wang[3], Wufeng Jiang[2], Chen Chen[1], Yuzhu Zhang[2], Jingbo Ren[1], Zhenguo Wang[1]

[1]North China University of Science and Technology Metallurgy and Energy College, Tangshan, China

[2]North China University of Science and Technology Qian'an College, Tangshan, China

[3]Institute of Power Source & Ecomaterials Science, Hebei University of Technology, Tianjin, China

Email address:

feng_lei2000@163.com (Lei Feng)
[*]Corresponding author

To cite this article:

Lei Feng, Fei Wang, Wufeng Jiang, Chen Chen, Yuzhu Zhang, Jingbo Ren, Zhenguo Wang. The Study on the Structure of Pure Iron Under a High Pressure of 100GPa. *Advances in Materials*. Vol. 6, No. 2, 2017, pp. 7-10. doi: 10.11648/j.am.20170602.11

Received: March 8, 2017; **Accepted**: March 16, 2017; **Published**: April 2, 2017

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

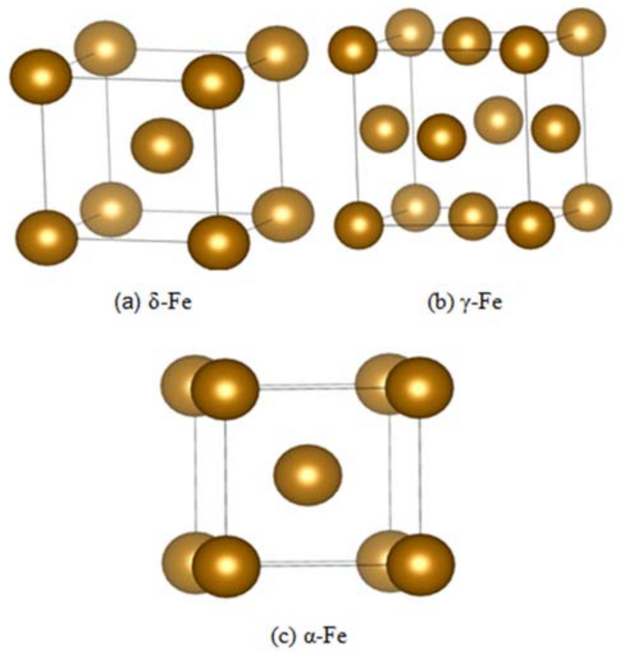

Figure 1. *The three allotropes of element Fe. (a) δ-Fe, (b) γ-Fe, (c) α-Fe.*

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 $2.28\mu_B$ of iron Fe.

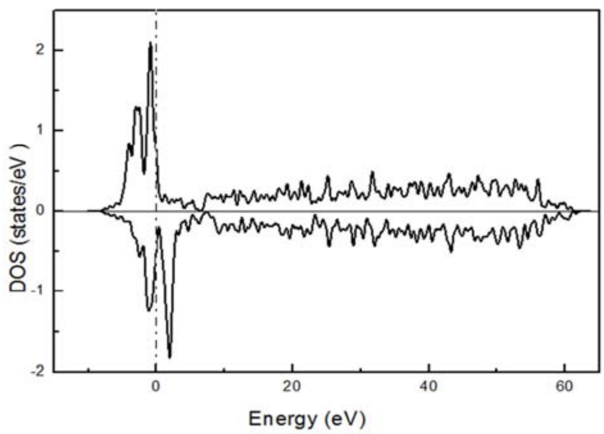

Figure 2. *The calculated total DOS for the structure of α-Fe.*

The spin-dependent energy bands along high-symmetry directions in the Brillouin zone for α -Fe are shown in Figure 3. It is obvious that there is no band gap, showing a conductor properties, most of the bands lies above the Fermi level, the bands energy range is from -10 eV to 65 eV, and at H, P and G high symmetry points in the Brillouin zone, band overlap obviously.

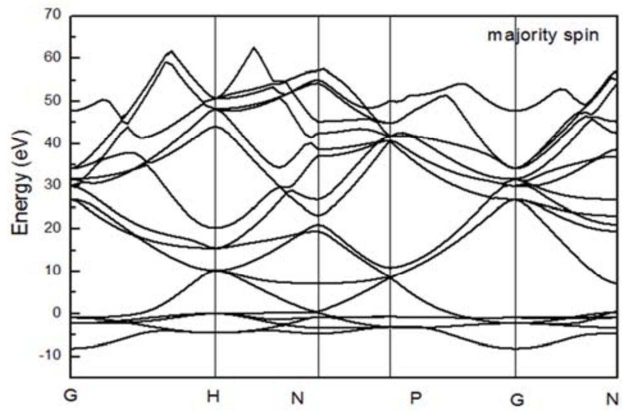

Figure 3. *Majority spin band structures for α -Fe. The zero of energy denotes the position of the Fermi level.*

Using the CALYPSO software, the structure of element Fe under 100GPa pressure has been studied. The results reveal that the *F*222 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, $\alpha=\beta=\gamma$

=90°. *F*222 is a 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.

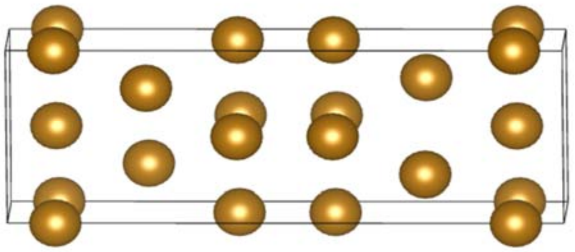

Figure 4. *The F 222 crystal structure of element Feunder 100GPa.*

The DOS of the structure *F*222 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 *F*222 which is also not a magnet, and the ferromagnetic property is dominated not by temperature but by high pressure.

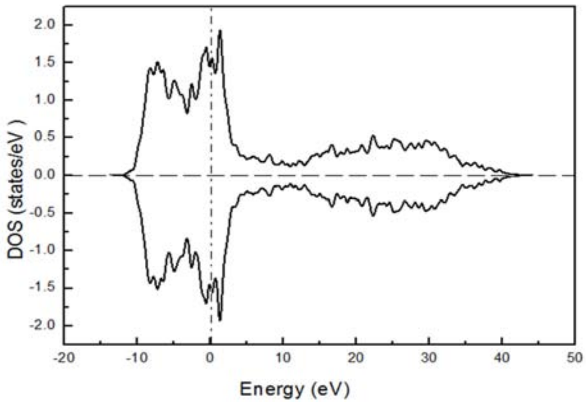

Figure 5. *Majority spin band structures for F222 of Fe. The zero of energy denotes the position of the Fermi level.*

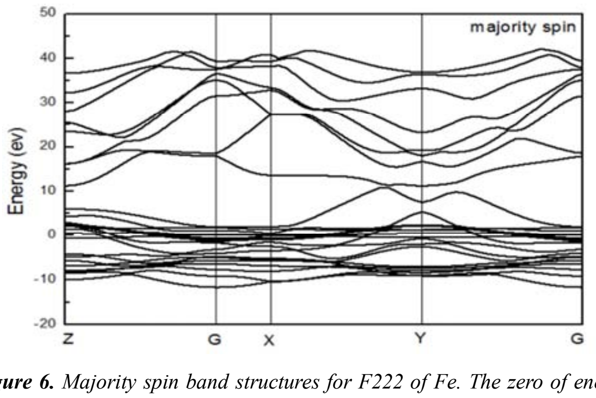

Figure 6. *Majority spin band structures for F222 of Fe. The zero of energy denotes the position of the Fermi level.*

The spin-dependent energy bands along high-symmetry directions in the Brillouin zone for F222 of Fe are shown in Figure6. One can see that the electric bands is very intensive around the Fermi level, showing which is a dense area of electrons, and this is also the result of the high pressure. The Fermi level crosses the valence band, so the element Fe with F222 structure shows conductive property.

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 *F*222 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.

Acknowledgements

The authors acknowledge the support by the Department of Science and Technology of Hebei Province (grant No: 15211034), China and the Innovation Project of University Student of North China University of Science and Technology Qian'an College, Tangshan, China.

This research was also supported by the National Natural Science Foundation of China (Grant no. 51404085), and the Key Technology R&D Program of Tianjin city (Grant no. 15ZCZDSF00030).

References

[1] Basinski, Z. s., Hume-rothery, W., Sutton, A. l. Proceedings of the Royal Society of London, Series A: Mathematical and Physical Sciences 76 (1955) 229.

[2] Bassett, W. a., Takahashi, T., Hokwang, Mao. Isothermal com pression of the alloys of iron up to 300 kbar at room temperature: Iron-nickel alloys. Journal of Physics and Chemistry of Solids, 25 (1964).

[3] Yanchao Wang, Jian Lv, Li Zhu and Yanming Ma, Phys. Rev. B. 82, (2010), 094116.

[4] Yanchao Wang, Maosheng Miao, Jian Lv, Li Zhu, Ketao Yin, Hanyu Liu, and Yanming Ma, J. Chem. Phys. 137, (2012), 224108.

[5] Shaohua Lu, Yanchao Wang, Hanyu Liu, Maosheng Miao and Yanming Ma, Nat. Commun. 5, (2014), 3666.

[6] Yanchao Wang, Jian Lv, Li Zhu, Shaohua Lu, Ketao Yin, Quan Li, Hui Wang, Lijun Zhang and Yanming Ma, J. Phys.: Condens. Matter. 27, (2015), 203203.

[7] Hui Wang, Yanchao Wang, Jian Lv, Quan Li, Lijun Zhang, Yan ming Ma, Comp. Mater. Sci. 112, (2016), 406.

[8] Yanchao Wang and Yanming Ma, J. Chem. Phys. 140, (2014), 040901.

[9] Chuanxun Su, Jian Lv, Quan Li, Hui Wang, Lijun Zhang, Yanchao Wang and Yanming Ma, J. Phys-Condens. Mat. (2017).

[10] Pengyue Gao, Qunchao Tong, Jian Lv, Yanchao Wang and Yanming Ma, Comput. Phys. Commun. 213, (2016), 40.

[11] J. Kennedy and R. Eberhart, IEEE. Piscataway. NJ. (1995), 1942.

[12] P. Hohenberg and W. Kohn, Phys. Rev. 136, (1964), B864

[13] E. Wimmer, H. Krakauer, M. Weinert and A. J. Freeman, Phys. Rev. B. 24, (1981), 864.

[14] M. Weinert, E. Wimmer and A. J. Freeman, Phys. Rev. B. 26, (1982), 4571.

[15] J. P. Perdew, J. A. Chevary, S. H. Vosko, A. Jackson, M. R. Pederson and C. Fiolhais, Phys. Rev. B. 46, 6671 (1992).