Tension and compression effect on mechanical properties of Fe and B2

Gang Huang, Qingdong Zhang and Shuo Li
School of Mechanical Engineering, University of Science and Technology Beijing, No. 30, Xueyuan Road, Haidian District, Beijing 100083, People’s Republic of China
E-mail: HGhuangAY@163.com

Keywords: stress-strain relationship, ideal strength, band structure, electronic density state

Abstract
The elastic constants, ideal strength, band structure and electronic density state of Fe and B2 under tension and compression were studied by using the first principle. The structural parameters calculated at 0 pressure are consistent with the experimental results. The dependence of elastic constant and stress can be obtained by using static finite strain technique. The ideal tensile and compressive strength of Fe and B2 were studied by calculating the stress-strain relationship. At last, the micro mechanism which affects the stability of the structure was analyzed by using the results of electronic structure calculation. The results show that the compressive strength of Fe and B2 structure is higher than the tensile strength. When the stress of cell structure exceeds a limit, it will be destroyed, resulting in the sudden decrease of Poisson’s ratio, $B$ and $G$, the asymmetry of energy band structure and the decrease of electron density of state energy.

1. Introduction

Silicon addition in steel has several profound effects. Due to the smaller atomic radius of Si (1.11 Å) than that of Fe (1.26 Å), the lattice parameter of Fe–Si decreases linearly with the increase of silicon content from 0 to 18 wt% [1, 2]. The decreasing slope changes at about 5 wt% of silicon content, which is related to the precipitation of order phase. Silicon addition rapidly increases the electrical resistivity of iron [2]. The magneto crystalline anisotropy also decreases with silicon addition [3], thus resulting in higher relative permeability of high silicon steel [4]. In addition to the main component Fe, silicon steel also contains three important Fe–Si phases: A2, B2 and DO3. Among them, the intermetallic compound B2 (FeSi) has attracted extensive attention of scholars in the past decades owing to the significant electrical and magnetic properties. At present, the functional applications of thermoelectric conversion and solar cells have aroused great interest [5, 6]. Among these compounds, the elastic property of B2 under high pressure and temperature has also attracted wide scientific attention due to the remarkable application in earth science [7–9]. Qi et al [10] studied the thermo elasticity of B2 under high pressure. Fischer et al [11, 12] studied the phase transition of B2 under high temperature and pressure. Moreover, the thermo elasticity and thermodynamic properties of B2 intermetallics were studied by using first-principles employing electronic DFT by Otero-de-la-Roza [3]. However, the related calculation result of mechanical properties of metals and their compounds are rarely reported up to now. Fe and B2 are both body centered cubic structures, of which ideal tensile and compressive strength and the differences of band structure and electron distribution should be further studied.

In this paper, the ideal strength of structure, elastic constants and band structure properties of Fe and B2 under pressure and tension state are researched. In addition, the stress-strain relation and deformation law of Fe and B2 are studied. All calculations in this paper are based on the first-principles plane-wave pseudo potential density function theory, which is realized in the Cambridge Serial Total Energy Package (CASTEP) [14].

© 2020 The Author(s). Published by IOP Publishing Ltd
2. Computational method

In this paper, the calculations were based on the density functional theory (DFT), generalized gradient approximation (GGA) \cite{15} and the Revised Perdew–Burke–Ernzerhof (RPBE) \cite{16} function were used. The ultrasoft pseudo potentials \cite{17} were used, and the cut-off energy for plane wave was set to 330 eV. The k-point mesh sampled in the Brillouin-zone were set as $4 \times 4 \times 3$ according to the Monkhorst–Pack \cite{18} scheme. The Brodyden–Fletcher–Goldfarb–Shanno (BFGS) \cite{19} minimization scheme was used in geometry optimization for each volume, which was considered to be completed when the total energy difference was less than $1 \times 10^{-5}$ eV/atom, Hellman–Feynman forces were less than 0.03 eV Å$^{-1}$, the maximum strain value was within 0.001 Å, and all of the stress components were within 0.05 GPa. When calculating the elastic modulus, the number of steps for each strain is set to 6.

In the calculation of tension and compression, a $2 \times 2 \times 2$ supercell structure of Fe and B2 is established, as shown in figure 1. In the pressure and tension calculations, the uniaxial tension and compression deformation was performed along the z direction in figure 2. The desired strains were set to a certain value while others were 0. The lattice vectors perpendicular to the strain direction and atomic positions were then relaxed simultaneously to obtain the equilibrium structures. We increased the desired strain step by step and repeated the above procedure. The minimum stress required for elastic instability of defect-free crystal is considered to be ideal tensile and compression strength \cite{20}.

3. Results and discussion

3.1. Structure

The equilibrium structural parameters of Fe and B2 are listed in table 1, as well as available experimental and other theoretical values. It is clear that our calculated values are in fairly good agreement with experiments values, so calculation results in this paper have good reliability.
3.2. Elastic properties

The complete knowledge of elastic parameters is crucial for understanding the mechanical behaviors of solids. To calculate the elastic constants, the finite-strain method compiled in the CASTEP code are used, in which a homogeneous strain of finite value is applied and then the resultant stress is calculated. The elastic constants are determined by solving the equation [23],

$$\sigma_{ij} = \sum_{ij} C_{ij} \varepsilon_{ij}$$  \hspace{1cm} (1)

The cubic system has three independent elastic constants, $C_{11}$, $C_{12}$ and $C_{44}$. Its mechanical stability criteria can be expressed as follows [24]:

$$C_{11} > 0, \quad C_{12} > 0, \quad C_{44} > 0, \quad C_{11} + 2C_{12} > 0$$  \hspace{1cm} (2)

The bulk modulus ($B$) and shear modulus ($G$) of polycrystalline aggregates were estimated from the individual elastic constants, $C_{ij}$, by the well-known Voigt [25] and the Reuss [26] approximations. The bulk modulus $B_V$ and shear modulus $G_V$ in the Voigt approximation are defined as:

$$B_V = \frac{(C_{11} + 2C_{12})}{3}$$  \hspace{1cm} (3)

$$G_V = \frac{(C_{11} - C_{12} + 3C_{44})}{5}$$  \hspace{1cm} (4)

In the Reuss approximation, the bulk modulus $B_R$ and shear modulus $G_R$ are defined as:

$$B_R = \frac{(C_{11} + C_{12} - 2C_{12}^2)}{3C_{11} - 3C_{12}}$$  \hspace{1cm} (5)

$$G_R = \frac{5C_{44}(C_{11} - C_{12})}{4C_{44} + 3(C_{11} - C_{12})}$$  \hspace{1cm} (6)

The actual effective moduli of anisotropic polycrystalline crystals can be obtained from the arithmetic mean of these two values as approximated by Hill [27]. In this approximation, the bulk modulus $B$ and shear modulus $G$ are given by:

$$B = \frac{1}{2} (B_R + B_V) \quad and \quad G = \frac{1}{2} (G_R + G_V)$$  \hspace{1cm} (7)

Again, the calculated bulk modulus $B$ and shear modulus $G$ allow us to estimate the Poisson’s ratio $\nu$ by the following relations:

$$\nu = \frac{3B - 2G}{2(3B + G)}$$  \hspace{1cm} (8)

The relationship between strain, bulk modulus and shear modulus of Fe and B2 unit cell structure was studied. As shown in figures 3–6, the results show that the curves of $B$ and $G$ change smoothly before the tensile and compressive strain of Fe unit cell reaches $\pm 0.15$, when the tensile and compressive strain reaches $\pm 0.15$, the curves of $B$ and $G$ change abruptly; the curves of $B$ and $G$ change smoothly before the tensile strain of B2 unit cell reaches 0.1 and the compressive strain reaches $-0.13$, when the tensile strain reaches 0.1 and the compressive strain reaches $-0.13$, the curves of $B$ and $G$ change abruptly. The results show that when the tensile and compressive strain of the Fe unit cell reaches $\pm 0.15$, the tensile strain of B2 unit cell reaches 0.1, and the compressive strain of B2 unit cell reaches $-0.13$, the unit cell structure suddenly changes, which may be the result of dislocations or phase transformations in the crystal after the strain exceeds the limit [28].

The relationship between strain and Poisson’s ratio of Fe and B2 unit cell structure was studied, and the results are shown in figures 7 and 8. It is generally believed the Poisson’s ratio is between 0–1, when The unit cell structure is in good condition. The Poisson’s ratio is negative, when the unit cell structure is destroyed. The results show that the structure is good, before the tensile and compressive strain of the Fe unit cell structure reaches $\pm 0.15$, and the Poisson’s ratio is between 0–1, the structure is damaged when the tensile and

| Type       | 0 GPa | Exp.               |
|------------|-------|-------------------|
| Fe         | 2.866 424 | 2.866(Fellinger et al) [21] |
| B2(FeSi)   | 2.748 952 | 2.773(Ono et al) [22]  |
Figure 3. The change of bulk modulus of crystal Fe in the process of tension and compression. (a) tension, and (b) compression.

Figure 4. The change of bulk modulus of crystal B2 in the process of tension and compression. (a) tension, and (b) compression.

Figure 5. The change of shear modulus of crystal Fe in the process of tension and compression. (a) tension, and (b) compression.
Figure 6. The change of shear modulus of crystal B2 in the process of tension and compression. (a) tension, and (b) compression.

Figure 7. The change of Poisson’s ratio of crystal Fe in the process of tension and compression. (a) tension, and (b) compression.

Figure 8. The change of Poisson’s ratio of crystal B2 in the process of tension and compression. (a) tension, and (b) compression.
compressive strain reaches ±0.15 and the Poisson’s ratio turns to negative. It is indicated that the structure is
good before the tensile strain reaches 0.1, the compressive strain reaches −0.13, and the Poisson’s ratio of B2
unit cell structure is between 0–1. And the structure is damaged when the tensile strain reaches 0.1. The
compressive strain reaches −0.13, and the Poisson’s ratio is negative.

3.3. Tension and compression properties
As shown in figures 9 and 10, the relationship between tensile and compressive stress and strain of Fe and B2 are
obtained. When the strain is low, the stress increases rapidly due to the high elastic modulus of Fe and B2. There
is a significant change occurred in the stress–strain curves at strain of Fe reaches ∼±0.15, the tensile strain of B2
reaches ∼0.1, and the compressive strain reaches ∼−0.13. The reason is that cell structure is destructed in which
case the maximum stress is considered to be the ideal tensile and compressive strength [29]. Therefore, the ideal
tensile strength and compressive strength of Fe are about 14.7 GPa and −34.4 GPa respectively. The ideal tensile
strength and compressive strength of B2 are about 23.7 GPa and −74.8 GPa.

As shown in the figures 9 and 10, whether for Fe or B2, the compressive strength is greater than the tensile
strength, which is about 2–3 times.

In conclusion, the relationship between strain and shear modulus, elastic modulus and Poisson’s ratio
proves that the structure of Fe unit cell is destroyed when the tensile and compressive strain are ±0.15. When the
tensile strain is 0.1 and the compressive strain is −0.13, the structure of B2 unit cell is destroyed. At the same
time, it is proved from figures 9 and 10 that the compressive strength of Fe unit cell structure and B2 unit cell
structure is higher than the tensile strength. Among them, the compressive strength of Fe unit cell structure is
about 2 times of the tensile strength, and that of B2 unit cell structure is about 3 times of the tensile strength. In
addition, the reason for the existence of steps in the iron compression stress-strain curve may be due to the transformation of the body-centered cubic into the close-packed hexagon. In this paper, taking Fe and B2 unit cells as examples, it is proved that the compressive strength of micro scale materials is higher than the tensile strength. The residual stress of materials measured by x-ray diffraction is calculated by the change of diffraction peak caused by the change of lattice constant. The calculation results in figures effectively explain which provides theoretical support for the detection and elimination of residual stress, that the residual stress measured by x-ray diffraction often gets larger compressive stress and rarely measures larger tensile stress which provides theoretical support for the detection and elimination of residual stress.

3.4. Band structure and Density of states
In this paper, the electronic structure is analyzed from two aspects: band structure and density of state. Energy band structure describes the energy of forbidden or allowed electrons, which directly reflects the distribution of valence band and conduction band. As a visual result of band structure the density of states can reflect the distribution of electrons in each orbit, and reveal the bonding situation inside the material. It can be seen from the figures that in the Brillouin region of Fe unit cell, the energy band distribution near the Fermi energy level (energy is 0) is overlapped. The energy bands of orbital localized electrons and
itinerant electrons occupy the vicinity of Fermi level. The energy band is bent and intersects with Fermi energy level without band gap region. From the structure and distribution of energy band, the shape of energy band has not been influenced by external force, that is to say, the metal characteristics of the system have not been changed. In the Brillouin region of B2 unit cell, when the unit cell structure is not destroyed, there are gaps in the band distribution near the Fermi energy level (energy is 0), the band is bent and does not intersect the Fermi energy level, There is a band gap region. When the unit cell structure is destroyed, the band gap disappears and the band intersects the Fermi level. The shape of energy band has been changed by external force, that is to say, the alloy characteristics of the system have been changed by external force.

As shown in figures 11–14, when the tensile and compression strain of Fe and B2 unit cells are 0 and ±0.03, the band structure shows good symmetry. When the tensile and compressive strain of Fe and B2 unit cells reach ±0.18, the band structure symmetry decreases, and both become asymmetric structures. The results show that when no plastic deformation occurs, the unit cell structure is intact and the band structure is symmetrical. When plastic strain occurs, the unit cell structure is destroyed, and the band structure becomes asymmetric.

In addition, the external force can changes the energy band distribution. With the increase of tensile stress, the energy bands on both sides of Fermi level move towards the Fermi level, indicating that the electronic energy near Fermi level increases gradually. With the increase of compressive stress, the energy bands on both sides of Fermi level move towards the direction away from Fermi level, indicating that the electronic energy near Fermi level decreases gradually.

From the electronic density of state, as show in figures 15, 16, it can be seen that the energy of Fe unit cell is higher, while that of B2 unit cell is lower, which shows that the activity of the whole unit cell is decreased by adding Si atom, and the whole structure tends to be the lower energy. When the unit cell structure is stretched, the electronic density of state energy shows an upward trend. When the unit cell structure is compressed, the electronic density of state energy shows a downward trend. When the unit cell structure is destroyed, the electronic density of state presents a multi peak state, and the electronic density of state hardly change.
It can be seen from the above figures 15–20 that with the increase of tensile stress, the peak and valley values of the distribution curve of spin electron density of state increase obviously near the Fermi level, indicating that the distribution number of spin electron near the Fermi level increase gradually, and the difference between the density of state of spin up and spin down moving electrons increase gradually. With the increase of the compressive stress, the peak and valley values of the distribution curve of the spin electron density of state decrease obviously near the Fermi level, which shows that the distribution number of the spin electron near the Fermi level reduce gradually, and the difference between the density of states of the spin up and spin down moving electrons decrease gradually. The properties of the system are affected directly by the distribution of spin electron density of state.
As shown in figures 17–20, the total density of states of the spin up and spin down of Fe unit cell is obviously asymmetric with respect to the energy axis, which leads to the obvious metal characteristics of Fe unit cell. While the total density of states of the spin up and spin down of B2 unit cell is obviously symmetrical with respect to the energy axis, which leads to the decrease of energy of B2 unit cell and metal characteristics. The results show that the addition of Si element greatly reduces the activity of the whole cell system.

Figures 21–23 shows the partial electronic density of states of Fe and B2 unit cells under different strains. It can be seen that the active contribution orbit of Fe atom is d-orbit, while the active contribution orbit of Si atom is p-orbit. And from the density of electronic states of Fe and B2 unit cells, the existence of Si greatly reduces the activity of Fe. At the same time, as figures 21–23 shows the energy of d-orbit of Fe atom and p-orbit of Si atom is higher when the strain is 0. When the strain is \( \pm 0.18 \), the structure is destroyed, and the energy of d-orbit of Fe atom and p-orbit of Si atom reduce rapidly. The results show that when plastic deformation occurs, the bonding strength is significantly reduced, and the structure is destroyed.
4. Conclusions

(1) In this paper, the first principle is used to calculate the stress and strain of single crystal Fe and B2 cells under uniaxial tension and compression. The results show the compressive strength is significantly higher than the tensile strength, about 2–3 times higher of the latter. This corresponds to the actual residual stress measured by x-ray diffraction, which proves that the results are scientific and provides a new idea for the study of micro residual stress.

(2) The structure, elasticity, ideal strength and deformation mode of Fe and B2 intermetallic compounds have been studied systematically and comprehensively by using electronic density functional theory. The state of good crystal structure and damaged crystal structure are compared and studied, and the calculated values are in good agreement with simulation results.

(3) The change laws of energy band structure and electronic density of state in the process of tension and compression were studied, the results show that in the process of tension and compression, once the strain exceeds the limit, the Fe–Fe and Fe–Si bonds will break, leading to plastic deformation of the crystal structure. In addition, the addition of non-metallic Si greatly reduces the activity of Fe. The addition of Si effectively improves the tensile and compressive properties of crystal structure.

Acknowledgments

This paper was supported by Beijing Natural Science Foundation (No. 3202019) and National Natural Science Foundation of China (No. 51575040).

ORCID iDs

Gang Huang 🐋 https://orcid.org/0000-0003-4992-1348
References

[1] Bozorth R.M and Ferromagnetism D 1951 *Van Nostrand Company* (New York: Van Nostrand) 849
[2] Miyazaki M, Ichikawa M, Komats T and Matsuda K 1992 Formation and electronic state of DO3-type ordered structure in sputtered Fe–Si thin films *J. Appl. Phys.* 71 2368–74
[3] Littmann M 1971 Iron and silicon–iron alloys *Iee T. Magn.* 7 48–60
[4] Callity B D and Graham C D 2011 *Introduction to Magnetic Materials* (New York: Wiley)
[5] Goiran F, Guyot P, Peyronneau J and Potier JP 1992 High-pressure and high-temperature reactions between silicates and liquid iron alloys, in the diamond anvil cell, studied by analytical electron microscopy *Journal of Geophysical Research: Solid Earth* 97 4477–87
[6] Maeda Y 2007 Semiconducting β-FeSi2 towards optoelectronics and photonics *Thin Solid Films* 515 8118–21
[7] Caracas R and Wentzcovitch R 2004 Equation of state and elasticity of FeSi *Phys. Rev. Lett.* 98
[8] Lin J F, Campbell A J, Heinz D L and Shen G 2003 Static compression of iron–silicon alloys: Implications for silicon in the Earth’s core *Journal of Geophysical Research: Solid Earth* 108
[9] Wann E, Vočadlo L and Wood I G 2017 High-temperature *ab initio* calculations on FeSi and NiSi at conditions relevant to small planetary cores *Phys. Chem. Miner.* 44 477–84
[10] Qi S, Zhang X, Niu Z, Liu C and Cai L 2019 First-principles investigations on elasticity properties of FeSi under high pressure and temperature *Physica B* 557 82–7
[11] Fischer R A, Campbell A J, Reeman D M, Miller N A, Heinz D L, Dera P and Prakapenka V B 2013 Phase relations in the Fe–FeSi system at high pressures and temperatures *Earth Planet. Sc. Lett.* 373 54–64
[12] Geballe Z M and Jeanloz R 2014 Solid phases of FeSi to 47 GPa and 2800 K: new data *Am. Mineral.* 99 720–3
[13] Otero-de-la-Roza A, Abbasi-Pérez D and Luaña V 2011 Gibbs2: a new version of the quasiharmonic model code. II. Models for solid–state thermodynamics, features and implementation *Comput. Phys. Commun.* 182 2332–45
[14] Segall M D, Lindan P J, Probert M A, Pickard C J, Hasnip P J, Clark S J and Payne M C 2002 First-principles simulation: ideas, illustrations and the CASTEP code *J. Phys. Condens. Matter* 14 2717
[15] Perdew J P, Burke K and Ernzerhof M 1996 Generalized gradient approximation made simple *Phys. Rev. Lett.* 77 3865
[16] Xu X and Goddard W A III 2004 The extended Perdew–Burke–Ernzerhof functional with improved accuracy for thermodynamic and electronic properties of molecular systems *J. Chem. Phys.* 121 4068–82
[17] Vanderbilt D 1990 Soft self-consistent pseudopotentials in a generalized eigenvalue formalism *Phys. Rev. B* 41 7892
[18] Monkhorst H J and Pack J D 1976 Special points for Brillouin-zone integrations *Phys. Rev. B* 13 5188
[19] F COMMER Z, G, CÔTE M, LOUIE S G and COHEN M L 1997 Relaxation of crystals with the quasi-Newton method *J. Phys. Chem. B* 101 233–40
[20] Zhang P, Meng F, Gong Z, Ji G, Yang J and Tang X 2014 Pressure and tension effects on mechanical properties of ZrAl2 AIP Adv. 4 117141
[21] Fellinger M R, Hector I G Fr and Trinkle D R 2018 Effect of solutes on the lattice parameters and elastic stiffness coefficients of body-centered tetragonal Fe *Comp. Mater. Sci.* 152 308–23
[22] Ono S, Kikegawa T and Ohishi Y 2007 Equation of state of the high-pressure polymorph of FeSi to 67 GPa *Phys. Chem. Miner.* 129 162–71
[23] Hadi M A, Kelaids N, Naqib H, Chrenvcs A and Isra A 2019 Mechanical behaviors, lattice thermal conductivity and vibrational properties of a new MAX phase Lu2SnC2 J. Phys. Chem. Solids 129 162–71
[24] Chong X, Jiang Y, Zhou R and Feng J 2014 First principles study the stability, mechanical and electronic properties of manganese carbides *Comp. Mater. Sci.* 87 19–25
[25] Voigt W 1928 *Lehrbuch der Kristallphysik* (New York: Teubner Leipzig)
[26] Reuß A 1929 Berechnung der dießgrenze von mischkristallen auf grund der plastizitätsbedingung für einkristalle *ZAMM-Journal of Applied Mathematics and Mechanics* 4 489–97
[27] Hill R 1952 The elastic behaviour of a crystalline aggregate *Proceedings of the Physical Society. Section A* 65 349
[28] Guo Y, Wang Y, Zhao D and Wu W 2007 Mechanisms of martensitic phase transformations in body–centered cubic structural metals and alloys: molecular dynamics simulations *Acta Mater.* 55 6634–41
[29] Zhou X, Qian G, Dong X, Zhang L, Tian Y and Wang H 2010 *Ab initio* study of the formation of transparent carbon under pressure *Phys. Rev. B* 82 134126
[30] Suzuki H 2020 Structural analysis and magnetic properties of lattice distortions from hexagonal to tetragonal systems in non-equilibrium Y–Fe alloys *Intermetallics* 119 106713
[31] Jiang W, Yu Y, Zhang W, Xiao C and Woo W 2020 Residual stress and stress fields change around fatigue crack tip: neutron diffraction measurement and finite element modeling *Int. J. Pres. Ves. Pp.* 179 104024
[32] Angerer P, Klünsner T, Morstein M and Gänser H 2019 Residual stress depth profiling of a coated WC-Co hardmetal-Part I of II: equi-penetration grazing incidence x-ray diffraction (EP-GIXD) method *Int. J. Refract. Met. Hard Mater* 83 104943