

Article

Mechanical Properties of DO3 Based on First Principles

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Abstract: The elastic constants, ideal strength, band structure and electronic density state of Fe₃Si (DO3) under triaxial tension and triaxial compression were studied using the first principle. The structural parameters calculated at zero pressure are consistent with the experimental results. The dependence of elastic constant and strain can be obtained using static finite strain technique. The ideal triaxial tensile and compressive strength of DO3 were studied by calculating the stress–strain relationship. The micro mechanism that affects the stability of the structure was analyzed using the results of electronic structure calculation. The results showed that the compressive strength of DO3 structure is higher than the tensile strength. When the stress of cell structure exceeds a limit, the covalent bond of Fe–Si is destroyed, resulting in the sudden decrease of *G* and *E* and the abnormal change of electronic density of state.

Keywords: stress–strain relationship; ideal strength; modulus of elasticity; band structure; electronic density state

1. Introduction

Silicon steel is a typical iron silicon alloy (Fe–Si). Due to its high conductivity, high temperature stability, soft ferromagnetism, and good oxidation resistance [1], silicon steel is widely used in aerospace, microelectronics, power and telecommunications engineering, and photoelectric fields [2–4], which has potential applications in the fields of solar cell devices, thermally stable contacts, cold tube light sources, magnetoresistive replacement devices, and spintronics devices. According to the phase diagram of Fe–Si alloy, a total of four kinds of Fe–Si compounds with different chemical ratios are formed in silicon steel, which are iron-rich phase Fe₃Si, mesophase Fe₅Si₃, monosilicide Fe–Si, and silicon-rich phase FeSi₂ [5,6]. Among them, Fe₃Si has excellent ferromagnetic properties and can be used as magnetic functional materials.

Fe₃Si (DO3) alloy is a typical body-centered cubic structure. It has excellent magnetic properties, corrosion resistance, oxidation resistance, and friction resistance. In addition, the two elements of Fe₃Si are abundant in the surface layer of the earth's crust, which makes Fe₃Si inexpensive and have broad prospects and applications in magnetic devices, microelectronics, and other aspects [7,8]. Cui et al. [9–11] showed that the cooling rate has an effect on the formation of Fe₃Si phase. Fu et al. [12] reported that in addition to the cooling rate, the deformation of the material has an effect on the Fe₃Si phase. Narita et al. [13] reported that Fe₃Si has the characteristics of low magnetostriction, high maximum permeability, and low coercivity. Scholars have studied the adsorption capacity, cohesive energy, heat formation, and acoustic properties of Fe₃Si [14–16], but there are few studies on mechanical properties of Fe₃Si.

The purpose of this study was to calculate the change in the mechanical properties of Fe₃Si (DO3) based on the first principles to, using Cambridge Serial Total Energy Package (CASTEP) code [17],

systematically study the relationship between strain and stress, and quantitatively study the difference between triaxial tension and triaxial compression. Based on the analysis of the change in the energy band structure and the density of electronic states, why such a change occurs will provide theoretical support for the study of the mechanical properties of microscopic materials.

2. Computational and Method

In this study, the calculations were based on the density functional theory (DFT), generalized gradient approximation (GGA) [18], and the Revised Perdew–Burke–Ernzerhof (RPBE) [19] functionals were used. The ultrasoft pseudo potentials [20] 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 $6 \times 6 \times 6$ according to the Monkhorst–Pack [21] scheme. The Brodyden–Fletcher–Goldfarb–Shanno (BFGS) [22] minimization scheme was used in geometry optimization for each volume, which is considered to be completed when the total energy difference is less than 1×10^{-5} eV/atom, Hellman–Feynman forces are less than 0.03 eV/Å, the maximum strain value is within 0.001 Å, and all of the stress components are within 0.05 GPa. When calculating the elastic modulus, the number of steps for each strain is set to 6. All the above calculations consider spin polarization.

In the calculation of tension and compression, a $2 \times 2 \times 2$ supercell structure of DO3 was established, as shown in Figure 1. In the pressure and tension calculations, the triaxial tension and compression deformation was performed along the x,y,z direction, as shown in Figure 2. The desired strains were set to a certain value while the 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 [23].

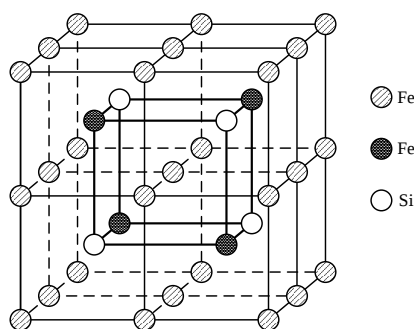


Figure 1. Schematic diagram of super cell structure of Fe₃Si (DO3).

The main components of silicon steel are Fe and Si, of which Fe accounts for more than 90%, followed by Si, which accounts for the most, while the other elements are negligible. There are three main Fe–Si phases in silicon steel [24,25]: A2, B2, and DO3, of which the A2 phase is a disordered phase, Fe and Si can be located anywhere in the system structure, B2 and DO3 phases are ordered, and Fe and Si have fixed positions. The crystal structure of DO3 studied in this paper is shown in Figure 1.

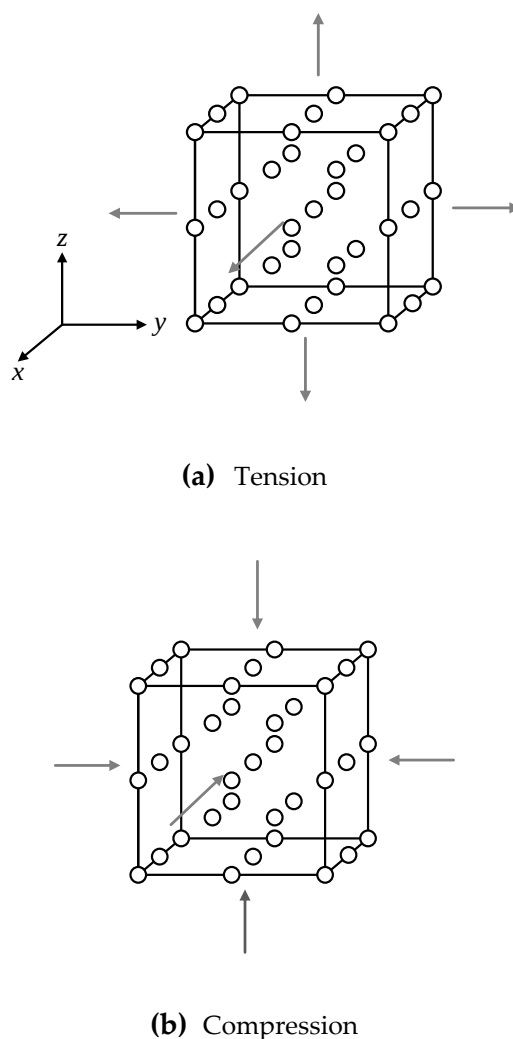


Figure 2. Schematic diagram of triaxial compression and tension of supercell. (a) Tension, and (b) compression.

3. Results and Discussion

3.1. Structure

The equilibrium structural parameters of DO3, as well as available experimental and other theoretical values, are listed in Table 1. Our calculated values were in fairly good agreement with experiment values, so the calculation results in this paper have good reliability.

Table 1. Lattice constants a , Young's modulus E and shear modulus B of DO3 intermetallic compound.

Contrast	a (Å)	E (GPa)	G (GPa)
Present	5.617513	232.6197071	88.41494
Exp.	5.630 [26]	228 [27]	88 [27]
Other	5.6550 [27]	242.12 [15]	

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 [28]

$$\sigma_{ij} = \sum_{ij} C_{ij} \varepsilon_j \quad (1)$$

where σ_{ij} is the stress tensor, C_{ij} is the elastic constant tensor, and ε_{ij} is the Lagrangian strain tensor.

The cubic system has three independent elastic constants: C_{11} , C_{12} , and C_{44} . Its mechanical stability criteria can be expressed as [29]:

$$\begin{aligned} C_{11} &> 0, C_{44} > 0 \\ (C_{11} - C_{12}) &> 0 \\ C_{11} + 2C_{12} &> 0 \end{aligned} \quad (2)$$

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 [30] and Reuss [31] approximations. The bulk modulus B_V and shear modulus G_V in the Voigt approximation are defined as:

$$B_V = \frac{(C_{11} + 2C_{12})}{3} \quad (3)$$

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

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

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

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

The actual effective moduli of anisotropic polycrystalline crystals can be obtained from the arithmetic mean of these two values as approximated by Hill [32]. In this approximation, the bulk modulus B and shear modulus G are given by:

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

Again, the calculated bulk modulus B and shear modulus G allow us to estimate Young's modulus E by the following relations:

$$E = \frac{9BG}{3B + G} \quad (8)$$

3.2. Elastic Properties

The relationship between the strain and shear modulus of the DO3 unit cell structure was studied. As depicted in Figure 3 the results show that the curves of G change smoothly and positively before the tensile strain of DO3 unit cell reaches 0.045 and the compressive strain reaches 0.19. When the tensile strain reaches 0.045 and the compressive strain reaches 0.19, the curves of G change abruptly. The results showed that when the tensile strain of DO3 unit cell reaches 0.045 and the compressive strain of DO3 unit cell reaches 0.19, the unit cell structure suddenly changes.

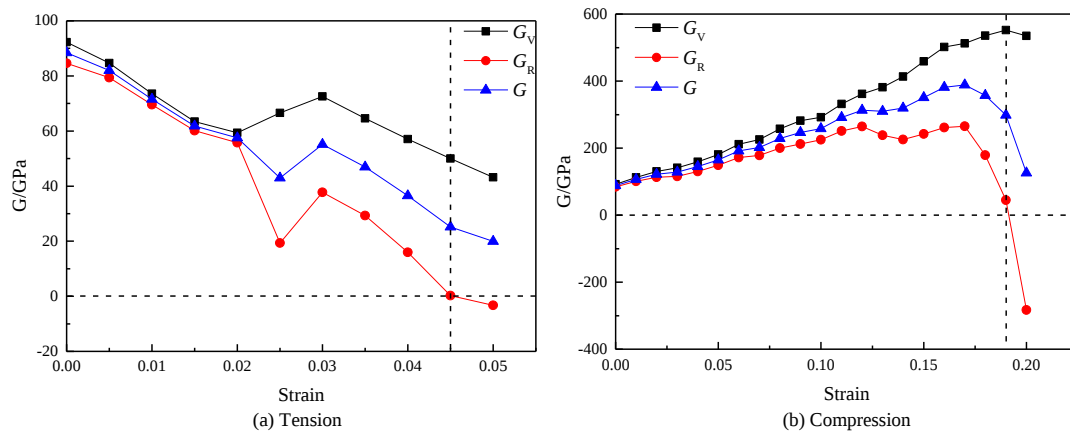


Figure 3. The change of shear modulus in the process of tension and compression. (a) Tension, and (b) compression.

The relationship between strain and Young's modulus of DO3 unit cell structure was studied, and the results are shown in Figure 4. It is generally thought that Young's modulus is positive when the unit cell structure is in good condition. Young's modulus is negative when the unit cell structure is destroyed. The results showed that the structure is good before the tensile strain reaches 0.045, the compressive strain reaches 0.19, and Young's modulus of DO3 unit cell structure is positive. The structure is damaged when the tensile strain reaches 0.05. The compressive strain reaches 0.2, and Young's modulus is negative.

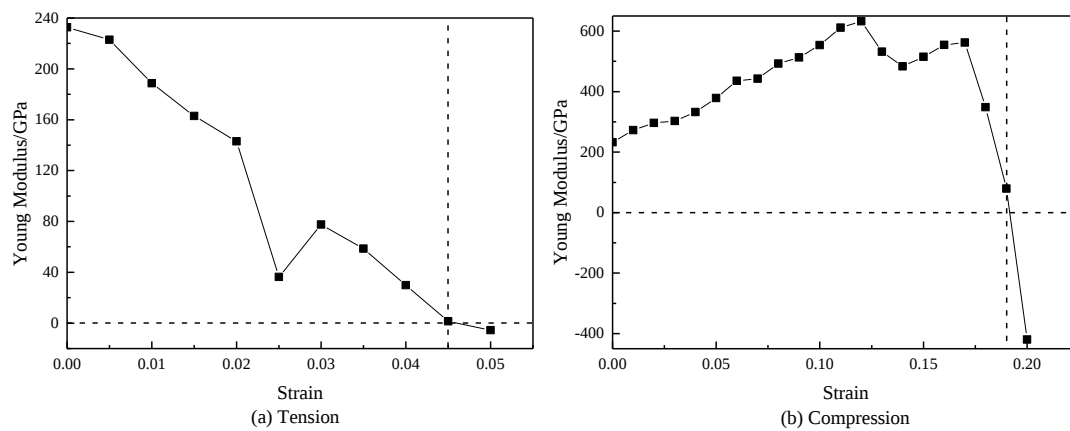


Figure 4. The change in Young's modulus in the process of tension and compression. (a) Tension, and (b) compression.

3.3. Tension and Compression Properties

As shown in Figure 5, the relationship between tensile and compressive stress and strain of DO3 was obtained. When the strain is low, the stress increases rapidly due to the high elastic modulus of DO3. A significant change occurs in the tensile strain of DO3 when it reaches ~0.05 and the compressive strain reaches ~0.2, at which point the cell structure is destroyed. Thus, the maximum stress is considered to be the ideal tensile and compressive strength [33]. Therefore, the ideal tensile strength and compressive strength of DO3 are about 17.0 GPa and −572.6 GPa, respectively.

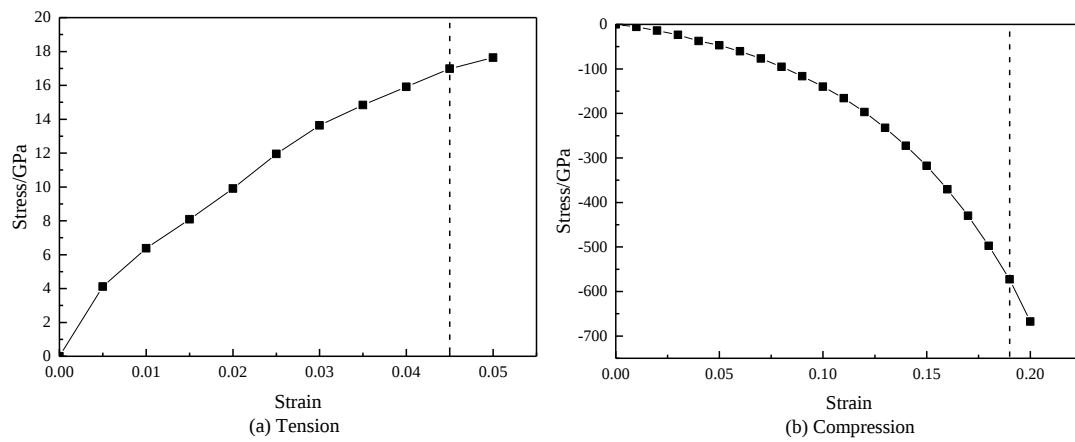


Figure 5. Stress–strain curve in the process of tension and compression. (a) Tension, and (b) compression.

In conclusion, in regard to the relationship between strain and shear modulus, Poisson's ratio proved that when the tensile strain is 0.045 and the compressive strain is 0.19, the structure of DO3 unit cell is destroyed. Figure 5 proves that the compressive strength of DO3 unit cell structure is higher than the tensile strength. Among them, the compressive strength of DO3 unit cell structure is about 33 times the tensile strength. Figure 6 shows that during the process of stretching and compressing the DO3 cell, the final energy of the crystal structure is constantly rising, indicating that the structure is becoming increasingly unstable.

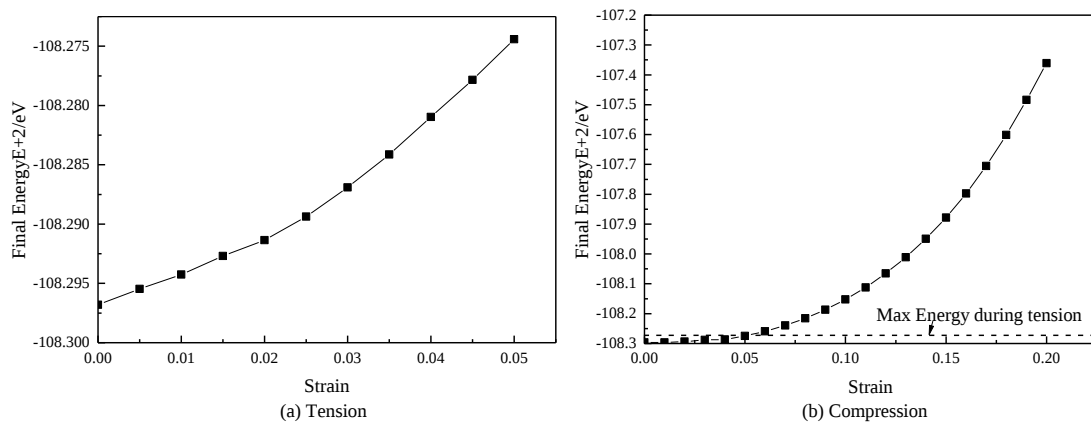


Figure 6. The change in energy in the process of tension and compression. (a) Tension, and (b) compression.

3.4. Band Structure

Figures 7 and 8 show that in the Brillouin region of DO3 unit cell, the energy band distribution near the Fermi energy level (energy is 0) is overlapped. The energy bands of the orbital localized electrons and itinerant electrons occupy the vicinity of the Fermi level. The energy band is bent and intersects with the Fermi energy level without a band gap. From the structure and distribution of the energy band, the shape of the energy band has not been influenced by external forces, that is, the metal characteristics of the system have not changed. However, the external force changes the energy band distribution. With the increase in tensile stress, the energy bands on both sides of the Fermi level move toward the Fermi level, indicating that the electronic energy near the Fermi level increases gradually. With the increase in compressive stress, the energy bands on both sides of the Fermi level move away from the Fermi level, indicating that the electronic energy near the Fermi level decreases gradually.

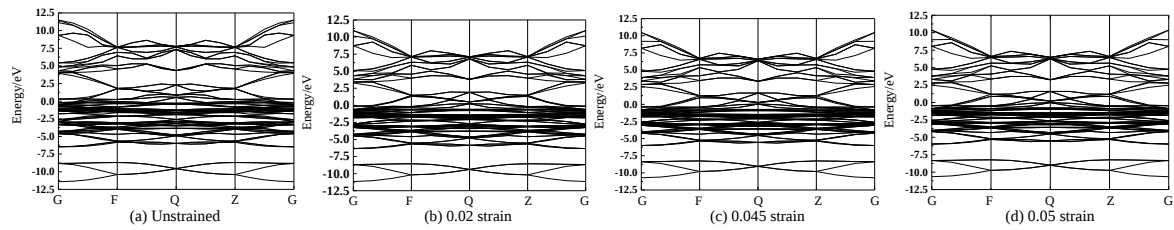


Figure 7. The change in band structure in the process of DO3 placed under triaxial tensile strains. (a) Unstrained, (b) 0.02 strain, (c) 0.045 strain and (d) 0.05 strain.

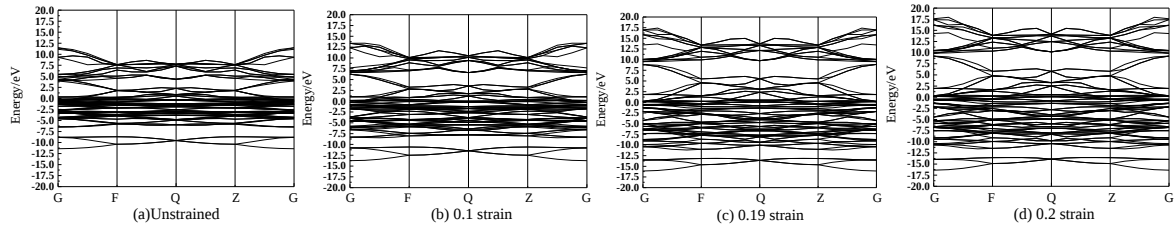


Figure 8. The change in band structure in the process of DO3 placed under triaxial compressive strain. (a) Unstrained, (b) 0.1 strain, (c) 0.19 strain and (d) 0.2 strain.

3.5. Electron Density

Figure 9 shows that with the increase in 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 electrons near the Fermi level increase gradually, and the difference between the density of state of spin up and spin down moving electrons increase gradually. Figure 9a shows that when the strain reaches 0.05, the peak height is significantly lower than that when the strain reaches 0.045. This change is inconsistent with the change law of the tensile process, indicating that the structure was damaged under this tensile strain state. With the increase in 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. This shows that the distribution number of the spin electrons 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. Figure 9b shows that when the strain reaches 0.2, the peak height is almost the same as when the strain is 0.19. This change is inconsistent with the change law of the tensile process, indicating that the structure was damaged under this tensile strain state. The properties of the system are affected directly by the distribution of spin electron density of state.

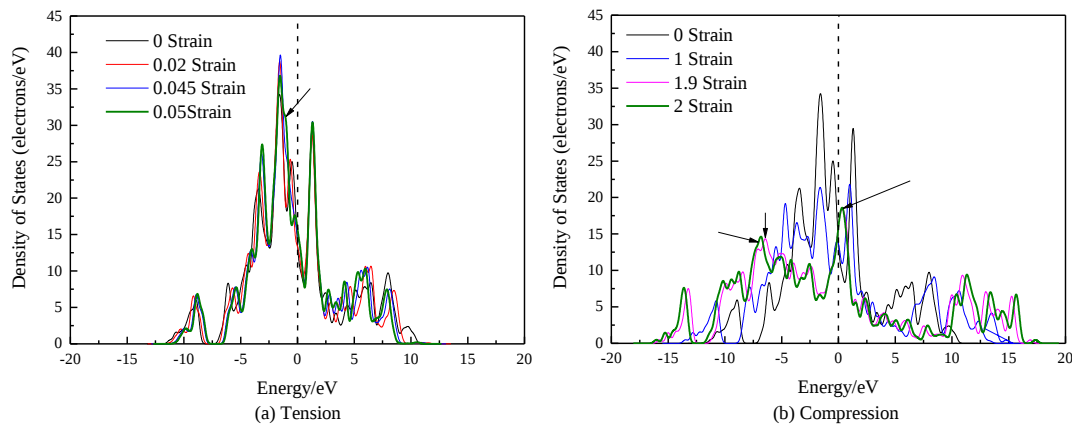


Figure 9. The change in electronic density of state in the process of tension and compression. (a) Tension, and (b) compression.

The deformation mode of this cubic structure was investigated. Figure 10 presents the valence electron density distribution in the (200) atomic plane of DO3 under triaxial tensile strains. Figure 10a shows the bonding situation before tensile strains were applied. There was strong covalent bonding of Fe–Si, and the bonding between Fe and Si atoms were mainly ionic. At first (Figure 10b), the Fe–Si bonds softened gradually under increasing triaxial tension; as the distance between the Si atom and the Fe atom increased, the attraction of the Si atom to the surrounding electrons of the Fe atom decreased, which made the electrons around the Fe atom more active. Thus, the weakening of Fe–Si led to the significant change at strain ~ 0.05 in Figure 9a. Figure 10c shows that with further increase in tensile strain, the electron density distribution of Fe–Si, which exhibits depletion, undergoes dramatic changes and eventually breaks (Figure 10d). In conclusion, the weakening and breaking of Fe–Si leads to the structural instability of DO3 under large tensile strains.

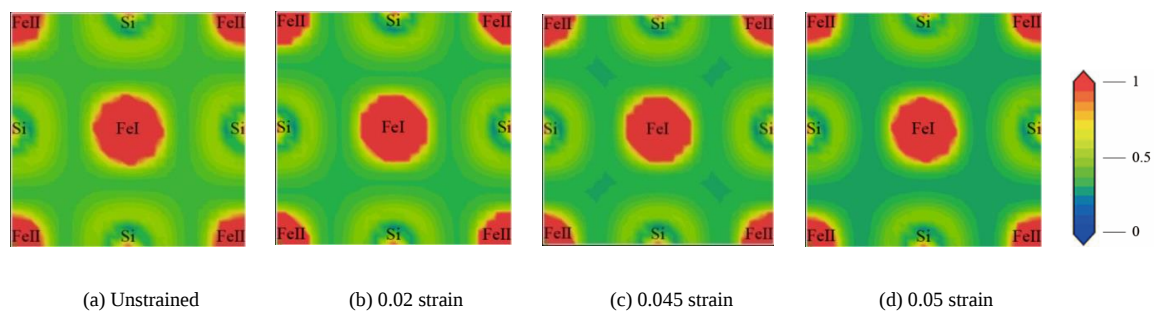


Figure 10. Valence electron density distribution in the (200) atomic planes of DO3 under triaxial tensile strains. (a) Unstrained, (b) 0.02 strain, (c) 0.045 strain and (d) 0.05 strain.

The deformation mode of this cubic structure was investigated. Figure 11 presents the valence electron density distribution in the (200) atomic planes of DO3 under triaxial compressive strain. Figure 12 shows the phonon dispersion distribution of the undamaged and damaged structure of DO3 under triaxial compression strain. Figure 11a shows the bonding situation before compressive strain was applied. For the same reason as tensile strain, there was strong covalent bonding of Fe–Si, and the bonding between Fe and Si atoms were mainly ionic. At the beginning (Figure 11b), the Fe–Si bonds enhanced gradually under increasing triaxial compression. When the distance between the Si atom and the Fe atom decreased, the attraction of the Si atom to the surrounding electrons of the Fe atom increased, which increased the electrons around the Si atom. When the distance is close to a certain extent, the attraction of the Si atom reaches a limit. At this time, the interaction between the Si atom and the Fe atom becomes repulsion, the covalent bond of Fe–Si is not strengthened, and the Fe–Si lattice is damaged under high pressure [34]. This led to the significant change at strain approximately 0.2 in Figure 9b. Figure 11c, with further compressive strain increase, the electron density distribution of Fe–Si, which exhibits depletion, undergoes dramatic changes and is eventually destroyed (Figure 11d). The phonon dispersion comparison chart of the undamaged structure and the damaged structure in Figure 12 shows that the phonon dispersion of the damaged structure significantly softened relative to the undamaged structure. Under high pressure, the crystal structure may produce a phase change and affect the stability of the structure, which is consistent with the conclusion previously stated [35]. In conclusion, the Fe–Si covalent bond destruction, lattice damage, and phase change leads to the structural instability of DO3 under large compressive strains.

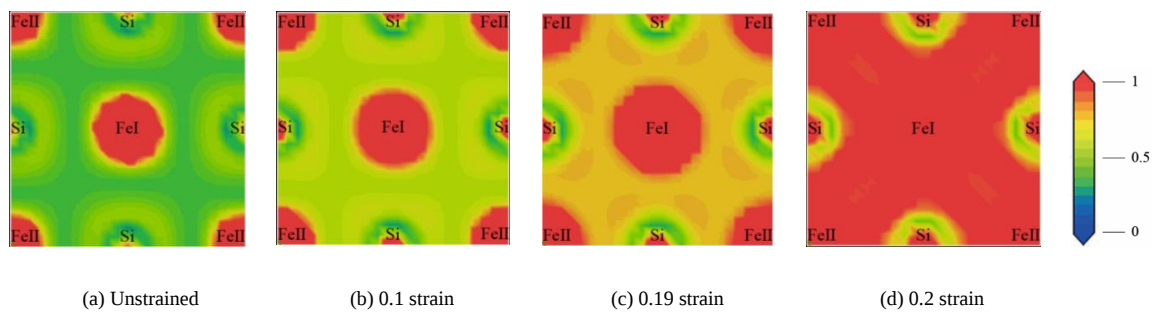


Figure 11. Valence electron density distribution in the (200) atomic planes of DO3 under triaxial compressive strain. (a) Unstrained, (b) 0.1 strain, (c) 0.19 strain and (d) 0.2 strain.

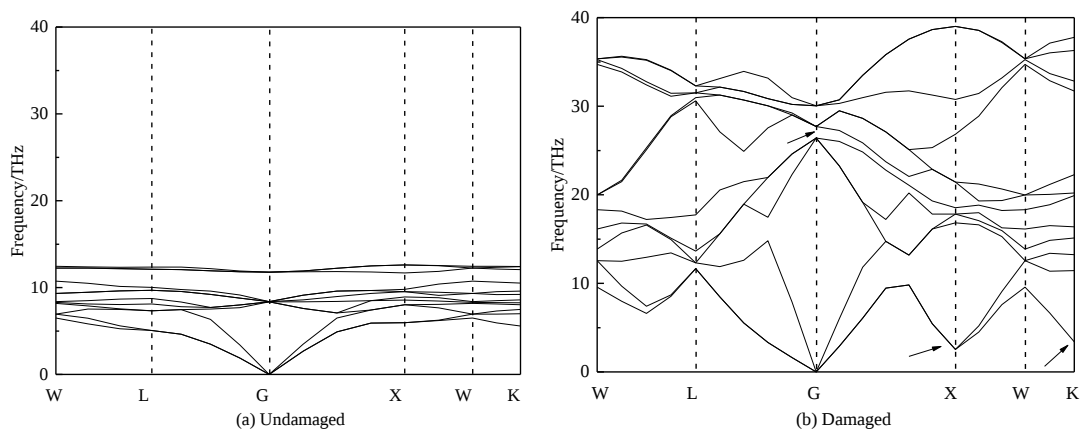


Figure 12. Calculated phonon dispersions of DO3 under triaxial compressive strain. (a) Undamaged, and (b) damaged.

4. Conclusions

(1) In this study, the structure, elasticity, ideal strength, and deformation mode of Fe_3Si (DO3) binary intermetallic compounds under the action of triaxial tensile and compressive deformation were systematically and comprehensively examined using electronic density functional theory. The findings provide theoretical support and new ideas for the study of mechanical properties of micro-scale materials.

(2) In this paper, the stress–strain relationship of DO3 cells under triaxial tension and compression were calculated using the first principle. The results showed that the triaxial compressive strength is significantly higher than the tensile strength, and the compressive strength is about 33 times the tensile strength. The state of the band structure and the electronic density of good and damaged crystal structure in the process of triaxial tension and triaxial compression were studied comparatively.

(3) The mechanism of strain-induced failure of crystal structure were analyzed from the law of electron distribution. The results showed that as the distance between Fe and Si atoms increases, the covalent bond of Fe–Si weakens during the tension process. With further stretching, the covalent bond of Fe–Si breaks, which leads to structural damage. During the compression process, the distance between Si atoms of the Fe nucleus decreases and the covalent bond of Fe–Si increases. When the covalent bond increases to a certain extent, the interaction between Fe and Si becomes repulsive, and the increase in strain leads to the destruction of the covalent bond, as well as lattice damage and phase change, which will cause structural damage.

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Conflicts of Interest: There is no conflict to declare.

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