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Research Article

Effect of (0001) Strain on the Electronic and Magnetic Properties of the Half-Metallic Ferromagnet Fe_2Si

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The electronic and magnetic properties of the half-metallic ferromagnet Fe_2Si under (0001) strain have been evaluated by the first-principles density functional theory method. The spin-up band structure shows that bulk Fe_2Si has metallic character, whereas the spin-down band structure shows that bulk Fe_2Si is an S-L indirect band gap of 0.518 eV in the vicinity of Fermi surface. Indirect-to-direct band gaps and an unstable-to-stable transition are observed in bulk Fe_2Si as strain is applied. In the range −11% to 11% (excluding zero strain), bulk Fe_2Si has stable half-metallic ferromagnetism, the spin polarization at the Fermi surface is 100%, and the magnetic moment of the Fe_2Si unit cell is 4.0 μB. The density distribution shows that the spin states of bulk Fe_2Si mainly come from the Fe^1-3d and Fe^3-3d states, indicating that bulk Fe_2Si has spin-polarized ferromagnetism. The half-metallic ferromagnetism of bulk Fe_2Si is mainly caused by d–d exchange and p–d hybridization, which are not sensitive to strain. It is very important to investigate the effect of changes in the lattice constant on the half-metallic ferromagnetic properties of bulk Fe_2Si.

1. Introduction

Half-metallic ferromagnets (HMFs) have attracted much attention because of their potential applications in spintronics [1]. Like a normal ferromagnet, HMFs have two different spin channels [2–4]. They have an energy gap in one spin direction at the Fermi level, whereas the other spin is strongly metallic, which results in complete spin polarization of the conduction electrons. Such materials generally have a high Curie temperature and close to 100% spin polarization [5, 6]. Therefore, half-metallic ferromagnetic materials will undoubtedly be an ideal semiconductor spin electron injection source. This shows that half-metallic ferromagnetic research is important and has application prospects. In addition, it will promote the rapid development of semiconductor spin electronics.

Bulk Fe_2Si has not been well investigated. Chen and Tan [7] used X-ray diffraction (XRD) to study the structure of Fe_2Si thin films. They found that the film thickness is affected by the base material, and the magnetic, electric, and optical characteristics are affected by the film structure. The structure, lattice parameter, phonon spectrum, and reflectance spectrum of hexagonal Fe_2Si have been investigated by first-principles calculations [8]. The results show that Fe_2Si is a ferromagnetic material and it has a spin-polarized half-metal-like band structure. However, there have been no studies associating the magnetism and mechanical properties of Fe_2Si. Therefore, in the present work, the properties of bulk Fe_2Si under (0001) strain were calculated using plane-wave pseudopotential methods based on density functional theory (DFT), and the results were analyzed in detail.

2. Calculation Method

There are four Fe atoms and two Si atoms in the Fe_2Si unit cell. The fractional coordinates of the three nonequivalent Fe atoms are (0, 0, 0), (0, 0, 0.5), and (0.333, 0.667, 0.78). The fractional coordinate of the Si atoms is (0.333, 0.667, 0.28). Fe_2Si belongs to space group $P-3m1$ (number 164). The lattice parameters are $a = b = 4.052$ Å and $c = 5.086$ Å. The crystal plane angles are $\alpha = \beta = 90^\circ$ and $\gamma = 120^\circ$. The (0001) strain line changes with the lattice constant c of the hexagonal Fe_2Si structure with strain ranging from −12% to 12%.

The calculations were performed with the plane-wave pseudopotential method implemented in the Cambridge sequential total energy package [9] to calculate the effect of (0001) strain on the electromagnetic mechanism of half-metallic ferromagnet Fe_2Si. The generalized gradient approximation [10] with the revised approximation of the Perdew–Burke–Ernzerhof scheme was used for the exchange–correlation potential. All of the possible structures were optimized by the Broyden–Fletcher–Goldfarb–Shanno algorithm [11, 12]. Geometry optimization was performed to fully relax the structures until self-consistent field (SCF) convergence per atom. The tolerance in the SCF calculation was 5.0×10^{-6} eV/atom. The ultrasoft pseudopotentials were expanded within a plane-wave basis set with 330 eV, and the iteration convergence accuracy was 5.0×10^{-7} eV. The energy of bulk Fe_2Si was calculated based on optimization of the structural system, with the minimum energy structure which was chosen as the stable structure. Sampling of the Brillouin zone (BZ) was performed with an $8 \times 8 \times 6$ k-point mesh according to the Monkhorst–Pack method [13].

3. Results and Discussion

3.1. Electronic Structure

3.1.1. Band Structure. Figure 1 shows the effect of (0001) strain on the band structure of bulk Fe_2Si near the Fermi energy. Figure 1(c) shows the band structure without strain. It shows that the band structure of spin-up electrons has metallic character and the band structure of spin-down electrons has semiconductor character. The valence band maximum is 0.164 eV at point S and the conduction band minimum is 0.682 eV at the BZ point L. Thus, Fe_2Si forms a band gap of 0.518 eV in the vicinity of Fermi surface (spin-down). The half-metallic gap [14] is determined by the minimum difference between the lowest energy of the spin conductive bands with respect to the Fermi level and the absolute value of the highest energy of the spin valence bands. Therefore, the half-metallic gap of bulk Fe_2Si is 0.164 eV.

Under (0001) plane strain, the lattice constant strain of bulk Fe_2Si changes its band structure, which leads to an energy change of the conduction band bottom and the valence band top. The valley near the bottom of the conduction band is divided into two groups of the degenerate valley, forming the conduction band edge and secondary conduction band edge. The energy shift of the valence band changes the light and heavy hole band into two groups of peaks, forming the valence band edge and the secondary valence band edge. The band gap (E_g) of the strain is determined by the heavy cavities and degenerate valleys. Figures 1(a) and 1(b) show the band structure of bulk Fe_2Si under compressive strain, which changes to a direct band gap of 0.338 eV at point L (spin-down). The strain reaches −12%; then bulk Fe_2Si becomes metallic. Figures 1(d)–1(f) show the band structure under tensile strain, which is the same as the band structure when applying compressive strain. This indicates that, under strain, bulk Fe_2Si is first a stable half-metallic ferromagnet and then changes to metallic with increasing strain. In conclusion, the band structure of bulk Fe_2Si can be changed using compressive and tensile strain, verifying that strain is an effective way to control the band structure.

3.1.2. Density of States. Figure 2 shows the total density of states (TDOS) and partial density of states (PDOS) of bulk Fe_2Si under various strains. The plotted energy range is −6 to 5 eV, and lower lying semicore states are omitted for clarity. Only the density of states (DOS) distribution near the Fermi level determines the magnetic properties. Hence, we concentrate on the DOS in the vicinity of the Fermi level, which is set to zero. To investigate the effect of strain on the subelectron structure of the system, the Si-s, Si-p, Fe-s, and Fe-d PDOS were investigated under various strains. The configuration of the extranuclear electrons of Si is $3s^2 3p^2$, and the configuration of the extranuclear electrons of Fe is $3d^6 4s^2$. Figure 2 shows that the DOS near the Fermi level mainly comes from Fe-3d spin states, and the contributions of Si-3p spin states are small. There is large exchange splitting between the spin-up and spin-down bands of the Fe-3d states, which leads to a large localized spin magnetic moment at the Fe atoms and results in polarization of the Fe-3d bands away from the Fermi level. Hybridization of 3p states provided by Si atoms with 3d electrons determines the degree of occupation of the p–d orbitals. Therefore, the half-metallic ferromagnetism of bulk Fe_2Si under various strains is mainly caused by d–d exchange and p–d hybridization.

The spin-up DOS is mainly distributed below the Fermi level. The spin-down DOS has two main peaks, which are located on both sides of the Fermi level. The spin-up and spin-down TDOS distributions near the Fermi surface are asymmetric; that is, the number of electrons in the spin-up and spin-down is quite different, which is the main contribution to the magnetic properties. Figures 2(b), 2(d), and 2(e) show that the Fermi level is completely located in the band gap of the spin-down energy band and the spin polarization of bulk Fe_2Si at the Fermi level is 100%, so the spin polarization of bulk Fe_2Si can be improved by strain.

3.2. Magnetic Properties

3.2.1. Magnetic Mechanism Analysis. The magnetic moments of all of the atoms in the Fe_2Si unit cell under various strains are given in Table 1. The total magnetic moment of the Fe_2Si unit cell under strains of −12%, −7%, 0%, 5%, 9%, and 12% are 9.29 μB, 4.01 μB, 3.54 μB, 4.00 μB, 4.00 μB, and 4.05 μB, respectively. This shows that bulk Fe_2Si has stable half-metallic ferromagnetism under strain of −11% to 11% (excluding zero strain), which agrees well with Figures 1 and 2. If half-metals are in the same applied magnetic field, larger magnetic moments possibly result in stronger spin-correlation scattering of conductive electrons, and the variation of the resistance is then larger. Therefore, bulk Fe_2Si under strain of −12% and 12% will have more magnetoresistance than under no strain. Table 1 shows that the magnetic moment of bulk Fe_2Si mainly comes from the Fe^1-3d and Fe^3-3d states.

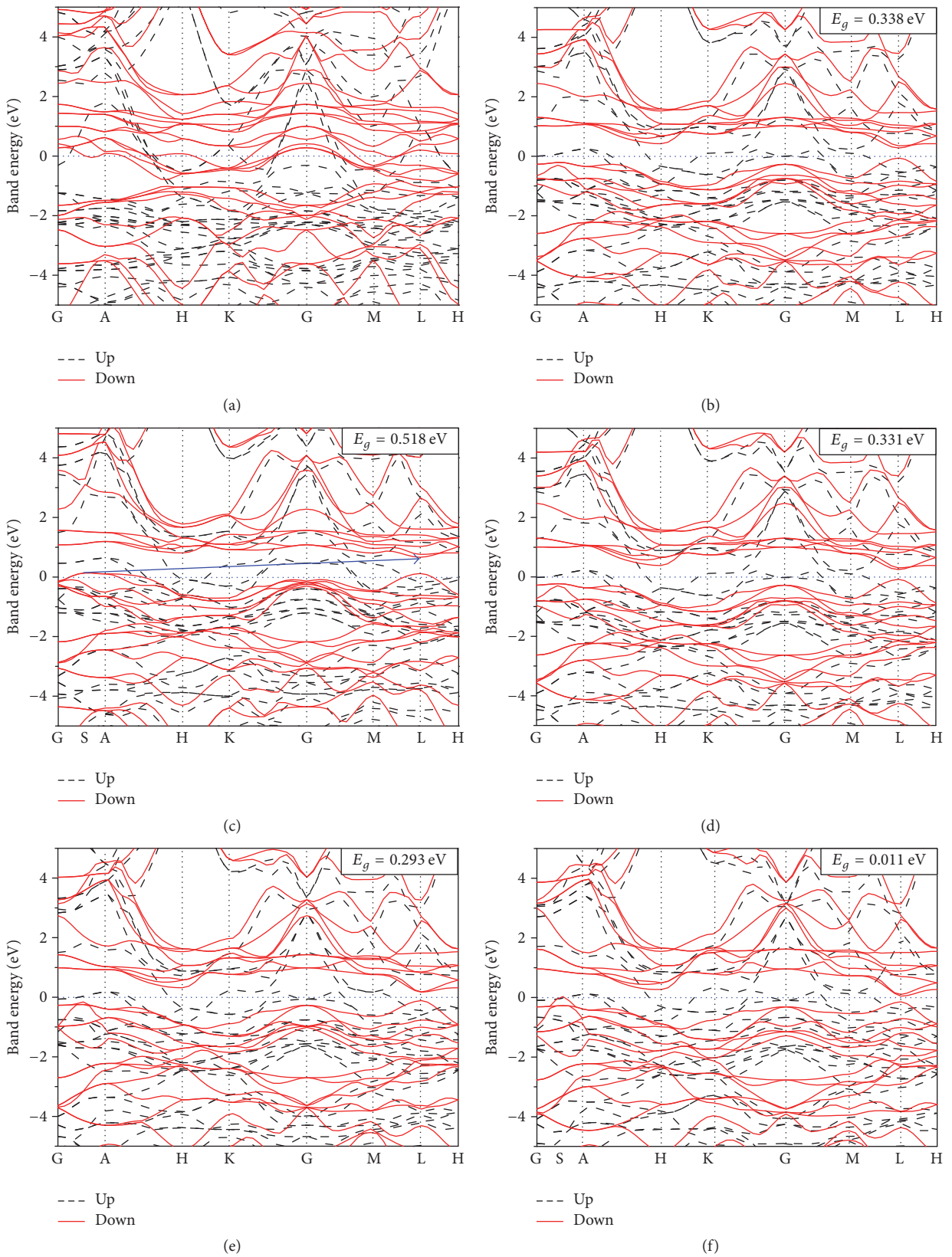

FIGURE 1: Band structures of Fe_2Si under various strains: (a) −12%, (b) −7%, (c) 0%, (d) 5%, (e) 9%, and (f) 12%. The band structure of spin-down electrons has indirect bandgap semiconductor character. The valence band maximum is 0.164 eV at point S and the conduction band minimum is 0.682 eV at the BZ point L. The blue arrow is from the top of the valence band point to the bottom of the conduction band.

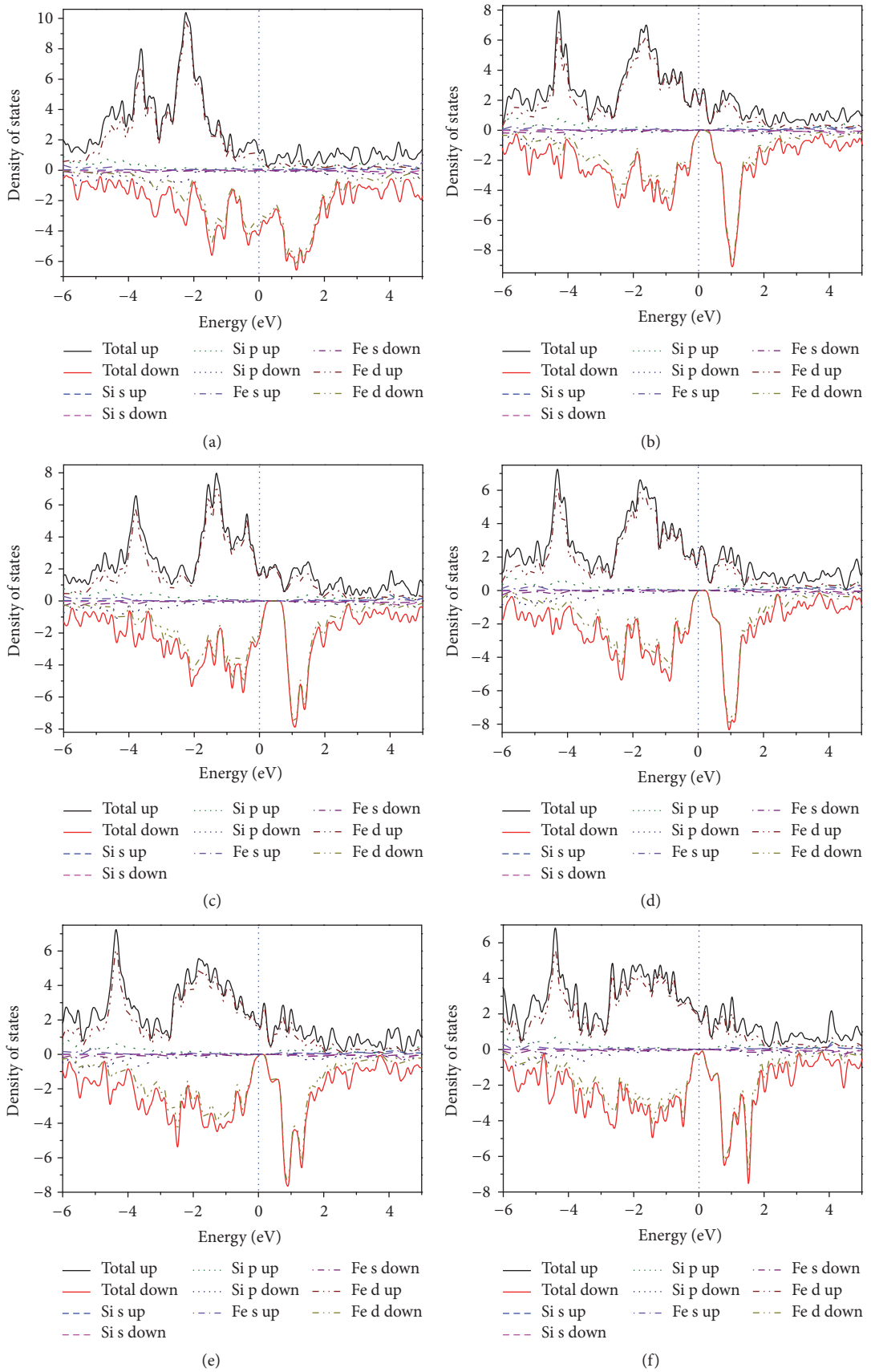

Figure 2: DOS of Fe_2Si under various strains: (a) −12%, (b) −7%, (c) 0%, (d) 5%, (e) 9%, and (f) 12%.

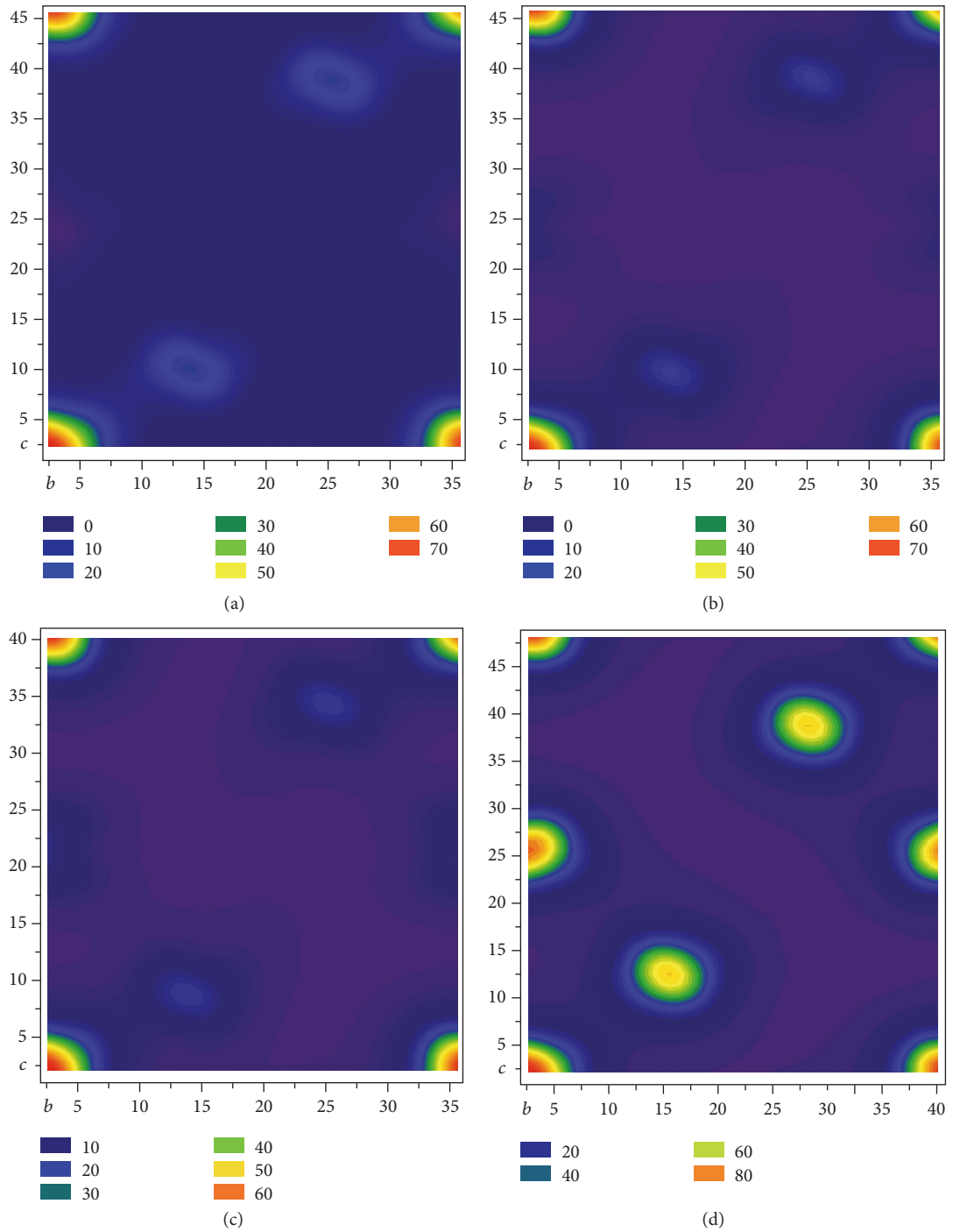

FIGURE 3: Spin density distributions of bulk Fe_2Si under various strains: (a) 0%, (b) −11% to 11% (excluding zero strain), (c) 12%, and (d) −12%.

In the range −11% to 11% (excluding zero strain), the total magnetic moment of bulk Fe_2Si is 4.0 μB and the spin polarization is 100% from the DOS map, indicating that the half-metallic ferromagnetic properties of bulk Fe_2Si are not sensitive to strain. In practical application in an optional electronic device, a small change in the lattice constant may have a significant effect on the electron transport properties at the Fermi level [15]. Therefore, it is very important to investigate the effect of changes in the lattice constant on the half-metallic ferromagnetic properties of bulk Fe_2Si.

3.2.2. Distribution of the Magnetic and Electric Charge. Figure 3 shows the spin density distributions of bulk Fe_2Si under various strains. The results show that the Fe atoms are surrounded by a high potential, whereas the Si atoms are surrounded by a low potential. The charge of Fe_2Si under

Table 1: Magnetic moments of all of the atoms in the Fe_2Si unit cell under various strains.

Species	Ion	−12% Spin (μB)	−7% Spin (μB)	0% Spin (μB)	5% Spin (μB)	9% Spin (μB)	12% Spin (μB)
Si	1	−0.34	−0.09	−0.06	−0.09	−0.09	−0.09
Si	2	−0.34	−0.09	−0.06	−0.09	−0.09	−0.09
Fe	1	2.81	2.83	2.80	2.81	2.75	2.69
Fe	2	2.58	0.06	−0.62	0.07	0.23	0.40
Fe	3	2.29	0.65	0.74	0.65	0.60	2.57
Fe	4	2.29	0.65	0.74	0.65	0.60	2.57

various strains is mainly localized on the Fe atoms and there is little charge on the Si atoms, indicating that bulk Fe_2Si has spin polarization ferromagnetism, which is consistent with the results in Table 1. The charge cloud distribution of the Si atom is affected by the Fe atom, making the distribution along the (11 $\bar{2}$ 0) crystal face. Charge transfer of the atoms in the system under stress is because of Fe d–d exchange and Fe-d–Si-p hybridization. In the range −11% to 11% (excluding zero strain), the charge density between atoms is relatively low. Figure 3 shows that the spin states of bulk Fe_2Si mainly come from the Fe^1-3d and Fe^3-3d states. Bulk Fe_2Si maintains its spin polarization ferromagnetism in the strain range.

4. Conclusion

The effect of (0001) strain on the electronic structure and magnetic properties of bulk Fe_2Si has been investigated by the first-principle pseudopotential method based on DFT. The spin-up band structure shows that bulk Fe_2Si has metallic character, whereas the spin-down band structure shows that bulk Fe_2Si is an S-L indirect band gap in the vicinity of Fermi surface. The half-metallic gap of bulk Fe_2Si is 0.164 eV. Applying strain, bulk Fe_2Si is first a stable half-metallic ferromagnet, and it then becomes metallic with further increasing strain. The DOS near the Fermi level mainly comes from Fe-3d spin states, and the DOS of Fe mainly comes from the Fe^1-3d and Fe^3-3d states, which are the source of the ferromagnetic properties of bulk Fe_2Si. The magnetic moment and charge transfer of bulk Fe_2Si are mainly caused by Fe d–d exchange and Fe-d–Si-p hybridization. In the strain range −11% to 11% (excluding zero strain), bulk Fe_2Si has stable half-metallic ferromagnetism and the spin polarization at the Fermi level is 100%, indicating that the spin polarization and half-metallic ferromagnetism of bulk Fe_2Si can be improved by strain.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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