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Study on the Electronic Properties of Silicon under Constant Voltage

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Abstract

In this paper, the electronic properties of silicon were studied by the first-principles methods at constant voltage. The research shown that the stress distribution along the crystal planes of (001), (101) and (111). The conduction band and valence band of Si shown anisotropy in the energy level and splitting energy at the G point of the band edge, sub band edge and secondary band edge. On the basis, we analyze the charge and bonding of Si material on [110], [101], [011], study the effect of changes in valence band structure on hole mobility, the results shown that the differential charge density is different on each surface, the intrinsic properties between the bonding method and the electronic structure. The calculation results provide data support and basis for the later research of silicon.

Keywords

Si, electronic structure, differential density of states, first principles method.

1. INTRODUCTION

In the 21st century, with the rapid development of all aspects of society, the innovation and replacement of materials have become very frequent [1]. Humans have increasingly higher requirements for photoelectric information, such as information, such as information storage, information transmission, and information processing [2]. Silicon as the first-generation semiconductor material, it had played a huge role in the fields of electronic information science and technology, such as semiconductor devices, aerospace detectors, photoelectric sensors, solar cells and other fields [3].

The microelectronics technology in the information age develops rapidly in accordance with Moor's law, but as the feature size is reduced to less than ten nanometers, whether the microelectronics industry can continue to advance in accordance with Moore's law is already facing challenges [4]. At this time, the smallest semiconductor unit-the size of the transistor's

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pole will reach 15nm, and electrons will traverse the channel by themselves trough quantum tunneling [5]. With the further improvement of IC integration, the power consumption and heat dissipation of the device will also restrict microelectronics technology [6]. So, the combination of microelectronics and optoelectronics, and give full play to the advanced and mature process technology, high-density integration and low price of silicon-based microelectronics, as well as the advantages of photonics extremely high broad band, ultra-fast transmission rate and anti-interference, have become the inevitability of information technology development and the general consensus of the industry.

The crystal structure of Si is mainly manifested in the periodicity and symmetry of the arrangement of microscopic atoms [7]. The symmetry and structure usually affect the physical and chemical properties of the crystal surface. The symmetry at the micro level will determine the symmetry at the macro properties, which shown the micro structure will be the decisive factor of the macro properties [8]. In this paper, the first-principles method is used to illustrate the influence of Si's charge distribution on its macroscopic performance from the electron distribution on each surface of Si.

2. CALCULATION METHOD

The electronic properties of silicon under constant voltage were studied by Frist principles method, all the calculations were executed using CASTEP (Cambridge serial total energy package) software package [9]. The interaction between lonic and electeonic interaction were calculated by Ultra Soft Pseudo Potential and Norm-conserving, respectively. The exchange-correlation potential was calculated by the PBE (Perdew Burker Emzerhof) of GGA (Generalized Gradient Approximation) method, the brillouin zone integration using Monkhorst-Pack method, the K-points was set as 4×6×3, the convergence accuracy was set 1×10^{-6}, all the calculation was in the reciprocal space.

3. RESULTS AND DISSCUSSION

3.1. The Electron Structure of Silicon

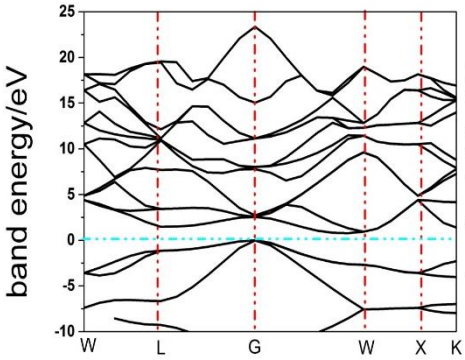

Fig 1. The band structure diagram of Si

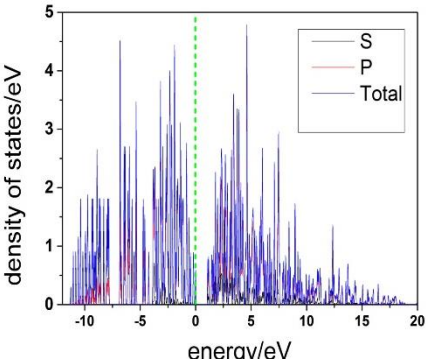

Fig 2. The density of states of Si

The figure 1 shown that Si is an indirect bandgap semiconductor, the maximum value of the valence band is 0eV at the point G, and the minimum value of the conduction band is 0.75eV at the point W. It can be see from the energy band diagram that there are degeneracy and splitting in the energy band of Si. The degeneration and splitting are different in different directions in the Brillouin zone. This indicates that Si is an anisotropic material, and electrons and holes have different mass in the Brillouin zone. The effective mass of Si in the Brillouin zone is different, and it is differently restricted by the potential field.

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The figure 2 is the density of states diagram. In the energy range of -13eV to -7.8eV, the density of states was mainly contributed by the S-orbital electrons of silicon. In the energy range of -6.5eV to -5eV, the density of states was mainly contributed by the S-orbital electrons of silicon, and the contribution of P-orbital electrons begins to increase. From -5eV to 0eV, the electron contributed by the p-orbital and s-orbital, but the contribution of p-orbital has surpassed the s-orbital, and the density of states was mainly contribution comes from the p-orbital electron transition. In the energy range of 0eV to -5eV, the density of states was mainly contributed by the p-orbital electrons jump.

3.2. The Electronic Properties of Silicon Under Constant Stress

3.2.1 The electronic properties of silicon under the (110) surface constant stress

Fig 3 is the difference in the density of states of Si, the electrical properties was changed by the changes of z axis in the (110) surface under the constant stress. In the figure, the blue area indicates a low potential, and the red area indicates a higher potential. The interconnecting lines in the image are the bonds between atoms. Along the thickness changes, the potential gradually decreases, and other areas are temporarily insignificant. With the change of the Z-axis direction in the high potential area, the potential gradually decreases and bonds are formed. Under the continuous change, the chemical bond begins to weaken, the low potential area expands, the original bond is broken, and the potential at the break increases. After that, the high potential starts to interact, there is a tendency to bond and the potential gradually decreases during the bonding process. Finally, the chemical bond was re-bonded.

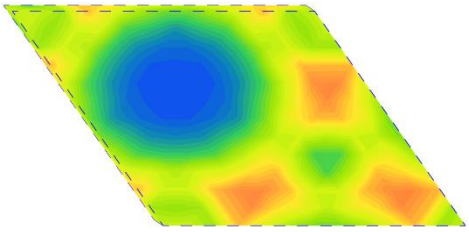

Fig a the differential density of states of Si(110)surface in 0.1 thinness

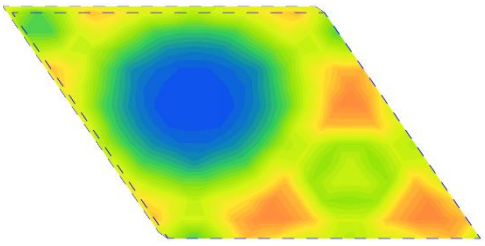

Fig b the differential density of states of Si(110)surface in 0.2 thinness

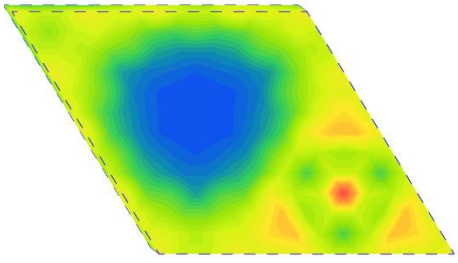

Fig c the differential density of states of Si(110)surface in 0.3 thinness

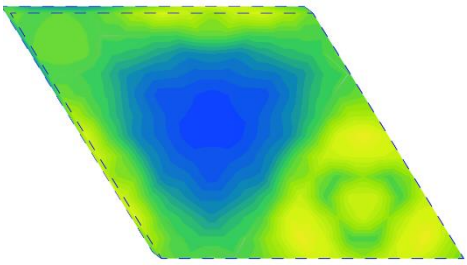

Fig d the differential density of states of Si(110)surface in 0.4 thinness

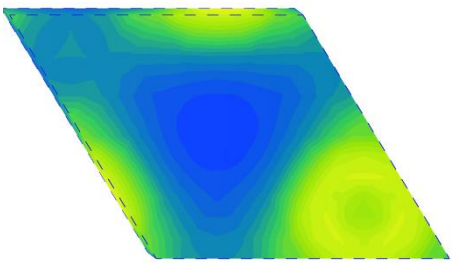

Fig e the differential density of states of Si(110)surface in 0.5 thinness

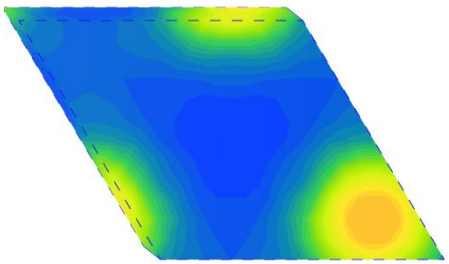

Fig f the differential density of states of Si(110)surface in 0.6 thinness

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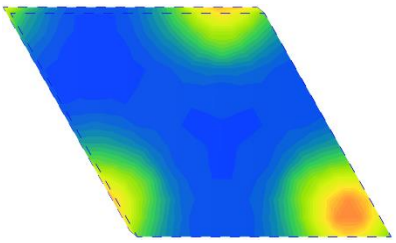

Fig g the differential density of states of Si(110)surface in 0.7 thinness

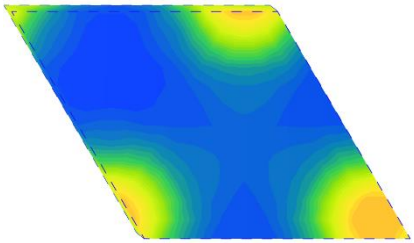

Fig h the differential density of states of Si(110)surface in 0.8 thinness

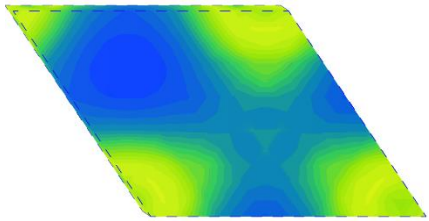

Fig i the differential density of states of Si(110)surface in 0.9 thinness

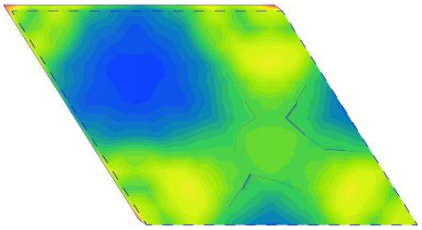

Fig j the differential density of states of Si(110)surface in 1.0 thinness

Fig 3. The differential density of states of Si(110)surface

3.2.2 The electronic properties of silicon under the (011) surface constant stress

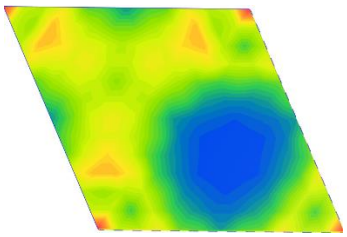

Fig a the differential density of states of Si(011)surface in 0.1 thinness

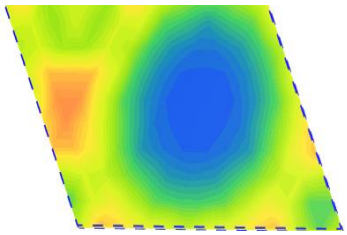

Fig b the differential density of states of Si(011)surface in 0.2 thinness

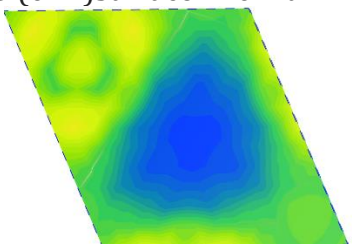

Fig c the differential density of states of Si(011)surface in 0.3 thinness

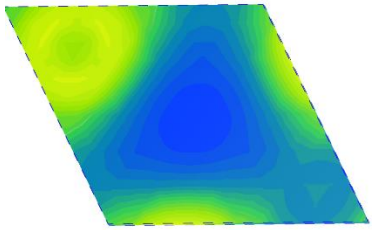

Fig d the differential density of states of Si(011)surface in 0.4 thinness

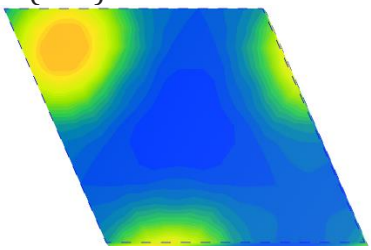

Fig e the differential density of states of Si(011)surface in 0.5 thinness

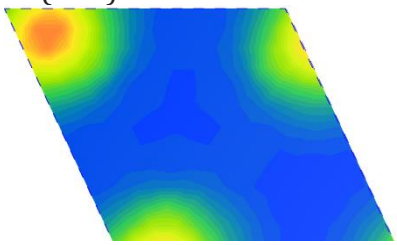

Fig f the differential density of states of Si(011)surface in 0.6 thinness

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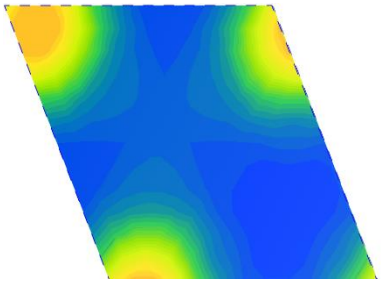

Fig g the differential density of states of Si(011)surface in 0.7 thinness

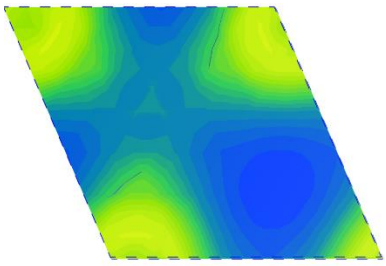

Fig h the differential density of states of Si(011)surface in 0.8 thinness

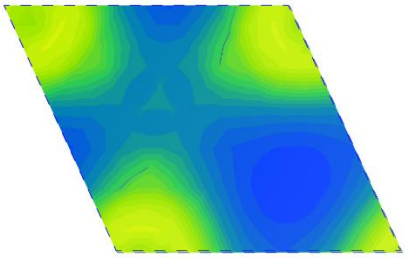

Fig i the differential density of states of Si(011)surface in 0.9 thinness

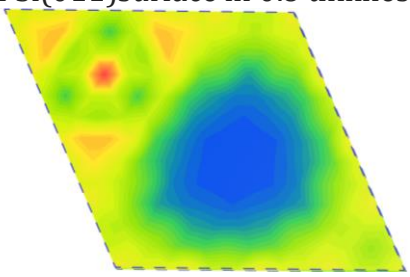

Fig j the differential density of states of Si(011)surface in 1.0 thinness

Fig 4. The differential density of states of Si(011)surface

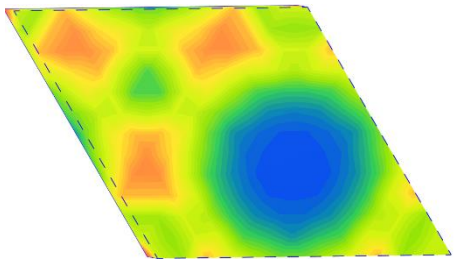

Fig a the differential density of states of Si(101)surface in 0.1 thinness

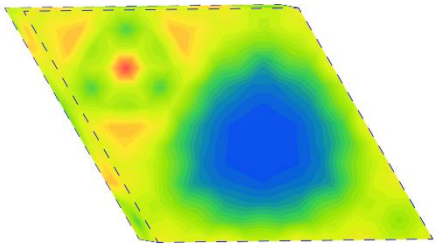

Fig b the differential density of states of Si(101)surface in 0.2 thinness

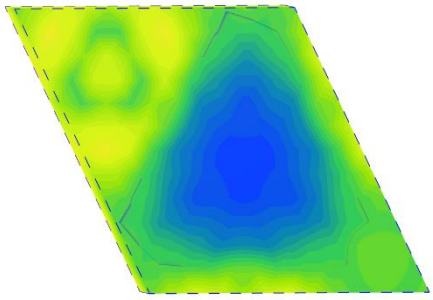

Fig c the differential density of states of Si(101)surface in 0.3 thinness

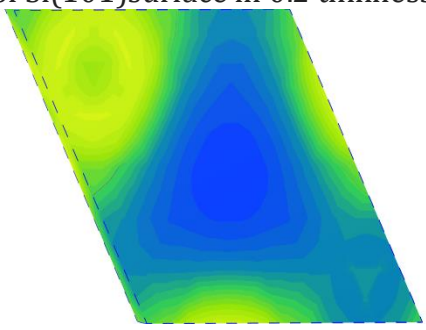

Fig d the differential density of states of Si(101)surface in 0.4 thinness

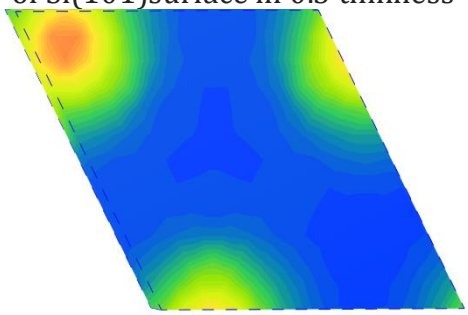

Fig e the differential density of states of Si(101)surface in 0.5 thinness

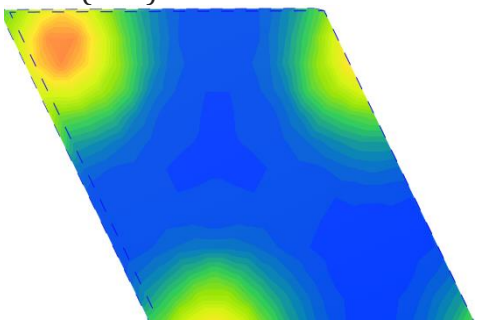

Fig f the differential density of states of Si(101)surface in 0.6 thinness

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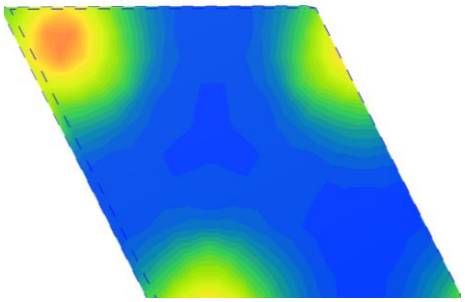

Fig g the differential density of states of Si(101)surface in 0.7 thinness

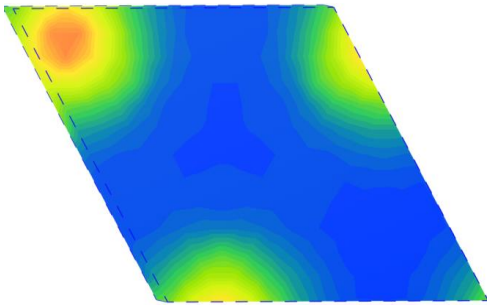

Fig h the differential density of states of Si(101)surface in 0.8 thinness

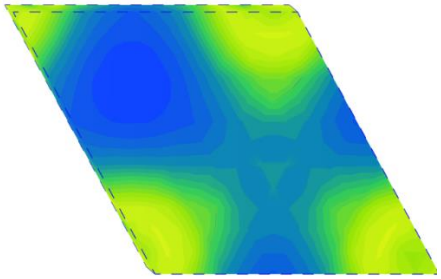

Fig i the differential density of states of Si(101)surface in 0.9 thinness

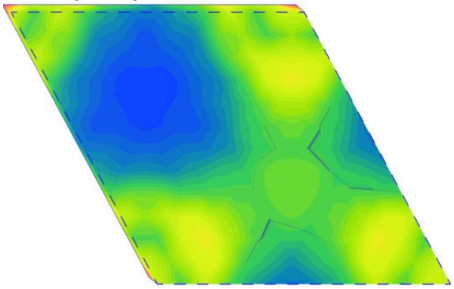

Fig j the differential density of states of Si(101)surface in 1.0 thinness

Fig 5. The differential density of states of Si(101)surface

Fig 4 is the difference in the density of states of Si, the electrical properties was changed by the changes of z axis in the (011) surface under the constant stress. In the figure, with the pressure changes in the X direction, the bond begins to break, and the potential at the break increases, and the area of the low potential was less change. Bonding was arise in the area where the potential rises, and the potential decreases during the bonding process. Since it acts on the system in the X direction, the potential rises in the corresponding direction. The high potential attracts each other and gradually has a tendency to bond in the X direction. When the pressure on the X axis peaks, the potential rises and bonds are formed, and it resulting to the chemical bond become strong.

3.2.3 The electronic properties of silicon under the (101) surface constant stress

Before it starts to change, it becomes a stable chemical bond. Under the directional pressure, the potential gradually decreases, and the bond energy becomes higher and higher. The potential continues to drop and the chemical bonds begin to break. The chemical bond breaks and the electric potential rises. Under the continuous increase of directional pressure, the interaction of high potentials begins to show a tendency of bonding. However, the keying in a specific direction oi offset, making it keyed in the initial direction of the Z axis. Analyzing the potential and bonding of silicon under pressure in various direction, combined with the differential density of states image, we can better grasp the electronic properties of Si.

4. CONCLUSION

In this paper, the electronic structure characteristics of Si were calculated by the first-principles method which based on the density functional theory under constant voltage. Analyze the energy band structure and electronic density of states image of Si and the differential density of states image of Si under different dimensional pressure. Under different direction pressure, the electronic structure and energy structure of Si will change to a certain extent, and the relative properties will also change macroscopically. Specifically, when the system is under pressure or influenced by external factors, it will cause the system structure

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including energy level transitions and electronic density of states to change. As a result, the system is modified and the original physical and chemical properties are lost.

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