MATEC Web of Conferences **227**, 01002 (2018) https://doi.org/10.1051/matecconf/201822701002
ICCT 2018

Molecular Dynamics Analysis of SiC Single Crystal Materials

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Abstract. SiC is modeled as a new generation of semiconductor materials because of its excellent properties. The 6H-SiC is modeled by Materials Studio. The band and state density of 6H-SiC are analyzed. In addition, 6H-SiC Substrate, the AL element doping, from the microscopic mechanism, analyzed the 6H-SiC semiconductor conductivity.

1 Introduction

SiC is a Group IV-IV semiconductor material. Because SiC has excellent properties such as large forbidden band width, high electron mobility and high thermal conductivity, it is an excellent semiconductor material for manufacturing high-power, high-frequency, high-temperature, anti-irradiation devices and The ideal material for optoelectronic integrated devices. SiC has a variety of homologous isomers, and its typical crystal structure is divided into two categories: one is a hexagonal or rhombic structure, with a large periodic structure such as 4H, 6H, 15R, etc., usually called α-SiC and the other is The cubic form of the zinc blende structure, commonly referred to as β-SiC. The general characteristics of various crystal forms of SiC are shown in Table 1:

Table 1. Characteristics of various SiC crystal forms

Performance	3C-SiC	2H-SiC
Molar mass(g * mol- 1)	40. 097	40. 097
Density(g *cm -3)	3. 22	3. 22
Melting point(℃)	2 730	2 730
Lattice constant(nm)	0. 43595	0. 3080
Dielectric constant	9. 72	10. 32
Breakdown electric field (V * cm-1)		
Electron mobility (cm 2* V-1 * s- 1)	1000	
Hole mobility (cm 2 * V-1 * s- 1)		40
Thermal conductivity (W* cm- 1 *K-1)	4. 9	4. 9
Electron saturation drift speed(cm * s- 1)	2. 0* 10^7	

In order to facilitate the comparison, we compare the performance of other natural forms of SIC in the form of a table. The comparison items we used include Breakdown electric field, Electron mobility, Hole mobility,Thermal conductivity and Electron saturation drift speed. The data of the comparison is shown in Table 2.

Table 2. Characteristics of various SiC crystal forms

Performance	4H-SiC	6H-SiC
Molar mass(g * mol- 1)	40. 097	40. 097
Density(g *cm -3)	3. 26	3. 03
Melting point(℃)	2 730	2 730
Lattice constant(nm)	0. 3073	0. 3073
Dielectric constant	9. 7	9. 7
Breakdown electric field (V * cm-1)	2. 2* 106	2. 4* 106
Electron mobility (cm 2* V-1 * s- 1)	1020	600
Hole mobility (cm 2 * V-1 * s- 1)	120	40
Thermal conductivity (W* cm- 1 *K-1)	4. 9	4. 9
Electron saturation drift speed(cm * s- 1)	2. 0* 10^7	2. 0* 10^7

2 Calculation methods and discussion

2.1 Molecular Dynamics Analysis of Intrinsic 6H-SiC Crystals

Materials Studio is a simulation software specially developed for materials science. The CASTEP module in Materials Studio uses advanced quantum mechanical algorithms. Therefore, Materials Studio is widely used in the electronic structure (energy band and density of states) of crystalline materials. Analysis, calculation of surface remodeling and its properties, lattice defects (grain boundaries, dislocations, etc.), charge density, semiconductor doping, etc. First, create a 6H-SiC model in the Materials Studio window, as shown in Figure 1:

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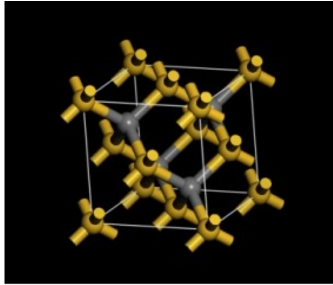

Figure 1. 6H-SiC model built in Materials Studio

First, the energy band diagram of the intrinsic 6H-SiC crystal is analyzed. The energy band diagram is shown in Figure 2:

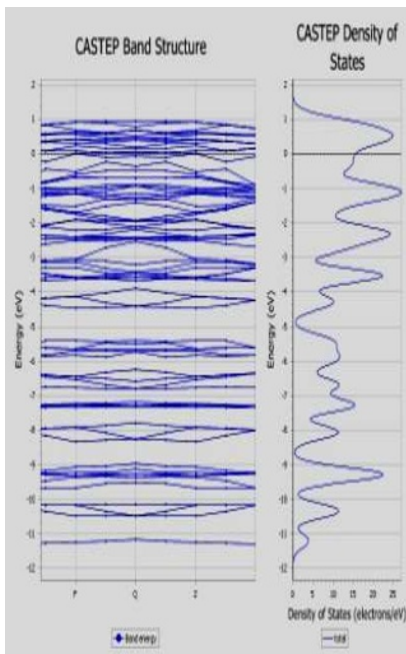

Figure 2. Energy band diagram of 6H-SiC

The energy band diagram analysis of 6H-SiC shows that the forbidden band width of 6H-SiC is calculated to be 2.5 eV, which is slightly narrower than the experimentally measured forbidden band width. The main reason is that the generalized gradient approximation (GGA) is used. When the 3D energy overestimation of 6H-SiC is caused, the energy overestimation tends to increase the 2p interaction between Si and C, which leads to the increase of the valence band bandwidth of 6H-SiC. low. However, the overall trend change of the 6H-SiC energy band diagram is consistent with the experimental values. It can be seen that the 6H-SiC band diagram calculated by the first principle, ie, the density functional theory can be used as the basis for analyzing the microscopic properties of 6H-SiC. It can also be seen from the energy band diagram that the lowest point of the conduction band and the highest point of the valence band are at the same symmetry point, which means that 6H-SiC is an excellent direct forbidden semiconductor material, and Figure 3 is 6H. -State density distribution map of SiC:

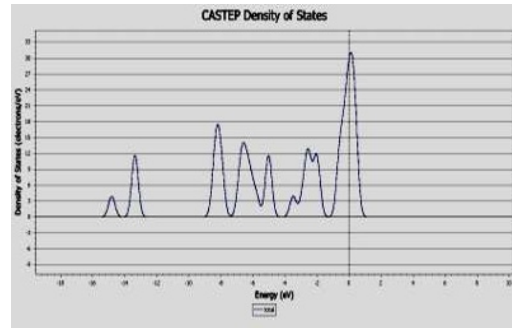

Figure 3. State density distribution of 6H-SiC

As can be seen from the analysis of Fig. 3, the density of states increases at the Fermi level, which indicates that the range of the Fermi level entering the valence band is deep. The N-type of 6H-SiC tends to be obvious. In Figure 3, the peak density of the p-electron of 6H-SiC is 25, and the peak density of the p-electron of 6H-SiC increases to 32, which means 6H-SiC. The phenomenon that the number of carriers does not match, the number of electrons is more than the number of holes, and then try to dope +3 valence elements, and judge whether the stability of the system and the performance of 6H-SiC performance.

2.2 Performance analysis after SiC doping

According to semiconductor theory, the electrical conductivity of a semiconductor material increases, which causes an increase in the dielectric constant. At the same time, it will also bring about an increase in dielectric loss and leakage. According to the principle of first matching after loss, 6H-SiC is used as the substrate material, and Al element is doped. FIG. 4 is a model diagram of doping Al element in 6H-SiC substrate:

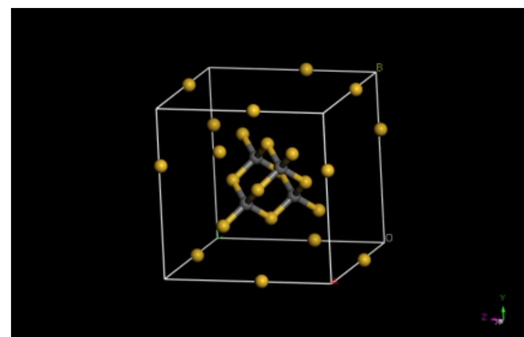

Figure 4. Doped Al in a 6H-SiC substrate

Energy band analysis of 6H-SiC doped with Al was carried out using the CASTEP module of Materials Studio. The energy band diagram is shown in Figure 5:

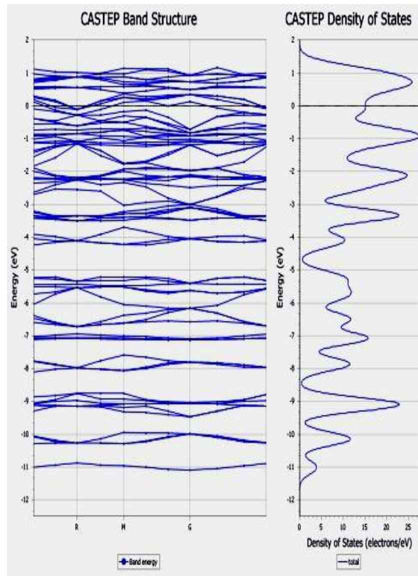

Figure 5. 6H-SiC band diagram of Al-doped element

The energy band diagram shown in Fig. 5 shows that after doping, the impurity level appears in the valence band, and the forbidden band width becomes wider. It can be seen from the analysis that the Fermi level has begun to enter the valence band. This means that intrinsic semiconductors have a tendency to shift toward p-type semiconductors. From the energy point of view, the energy of the system has improved. From the point of view of electronic structure, in the impurity semiconductor, Ef enters the valence band, and the quantum state near the end of the valence band terminus has been substantially occupied by the hole, which means that the doping level is high. Next, we analyze the state density map of the doped Al element. The density distribution of the 6H-SiC state doped with Al is shown in Figure 6:

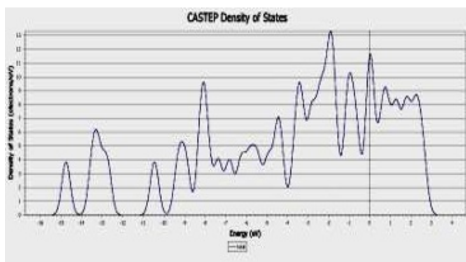

Figure 6. Density distribution of 6H-SiC state doped with Al

It can be seen from the analysis of Fig. 6 that the doping composition has a certain influence on the electrical conductivity of 6H-SiC. We use the electrons of the 3d, 4s and 4p states of the Al atom as valence electrons, and the 2s and 2p electrons of 6H-SiC as valence electrons for comparative analysis. Since 6H-SiC crystals have certain lattice defects, they are Multiple donor states are generated on the density distribution map, while Al is easier to compensate for the N impurity acceptor for the preparation of p-type doped 6H-SiC, so Al is a better dopant.

3 Calculation

Crystal growth can be considered to be caused by stable electrical oscillation, assuming that the growth of the container length is l, voltage is $v_0 \sin \omega t$, the problem can be described as:

$$E_{tt} - a^2 E_{XX} = 0 \tag{1}$$

$$E\,|_{X=0} = v_0 \sin \omega t \tag{2}$$

$$E\,|_{X=l} = 0 \tag{3}$$

Because the use of complex numbers to calculate more convenient, Therefore, the boundary condition $v_0 \sin \omega t$ is rewritten as $v_0 e^{i\omega t}$, that is, the imaginary part of the complex number $\mathrm{Im}(v_0 \sin \omega t)$. When the calculation is completed, the imaginary part of the result is the solution of the equation. Since the steady oscillation is caused by the AC power supply, the cycle is the same as the AC power cycle:

$$E(x,t) = X(x) e^{i\omega t} \tag{4}$$

Substituting equation (4) into the ordinary differential equation of X yields: $X'' + (\omega / a)^2 X = 0$

Solving the ordinary differential equation of X: $X(x) = Ae^{\frac{i\omega x}{a}} + Be^{-\frac{i\omega x}{a}}$, and so:

$$E(x,t) = \left[Ae^{\frac{i\omega x}{a}} + Be^{-\frac{i\omega x}{a}} \right] e^{i\omega t} \tag{5}$$

Substituting equation (5) into equation (2) yields:

$$[A + B] e^{i\omega t} = v_0 \sin \omega t \tag{6}$$

Substituting equation (5) into equation (3) yields:

$$\left[Ae^{\frac{i\omega l}{a}} + Be^{-\frac{i\omega l}{a}} \right] = 0 \tag{7}$$

The imaginary part of expression $E(x,t)$ is the final solution of the equation:

$$E(x,t) = v_0 \frac{\sin \frac{\omega(l-x)}{a} \sin \omega t}{\sin\left(\frac{\omega l}{a}\right)} \tag{8}$$

Assuming that there is an initial perturbation in region, the region affected by this disturbance can be described as a sphere with the center of M as the radius and the sphere as the inner envelope and the outer The surface of the surface is the area where the fluctuation has been conveyed, and the outer envelope is the area where the

disturbance has not yet been conveyed. The above process is described by the following equation:

$$E_{tt} - a^2 \Delta E = 0 \quad (9)$$

The equation is implemented by separating the variable method:

$$E(r,t) = T(t)v(r) \quad (10)$$

Equation (10) is substituted into equation(9): $\frac{T''}{a^2 T} = \frac{\Delta v}{v}$

Equation on the left is a function of t ,the right side of the equation is a function of r, the equation to be established, must be equal to the same constant, the constant as $-k^2$, then get two equations:

$$T'' + k^2 a^2 T = 0 \quad (11)$$

$$\Delta v + k^2 v = 0 \quad (12)$$

The solution of Eq. (11) is:

$$\begin{cases} T(t) = C\cos kat + D\sin kat & (k \neq 0) \\ T(t) = C + Dt & (k = 0) \end{cases}$$

In the spherical coordinate system, the solution of Eq. (12) is:

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(\frac{r^2 \partial v}{\partial r}\right) + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2 v}{\partial \varphi^2} + k^2 v = 0 \quad (13)$$

Separate variables on variable V：

$$v(\rho,\varphi,z) = R(\rho)Y(\theta,\varphi)$$

Substituting equation (13)，Equation (13) is divided by $\left(\frac{r^2}{RY}\right)$ at both ends：

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + k^2 r^2 = \frac{-1}{Y\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) - \frac{\partial^2 Y}{\partial\varphi^2}$$

The left side of the equation is a function of r, and the right side of the equation is a function of θ and φ. If the equation holds, the equation needs to be equal to a constant Let the constant be $l(l+1)$:

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) = \frac{-1}{Y\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) - \frac{R}{Y\sin^2\theta}\frac{\partial^2 Y}{\partial\varphi^2} = l(l+1) \quad (14)$$

Get two equations :

$$\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{\partial^2 Y}{\partial\varphi^2} + l(l+1)Y = 0 \quad (15)$$

Equation (14) is not a standard Bessel equation, and the equation (14)is transformed so that: $x = kr$, Substituting equation (14)

$$x^2 R'' + 2xR' + \left[x^2 - l(l+1)\right]R = 0 \quad (16)$$

Let $R = \frac{\omega}{\sqrt{x}}$, substitute equation (14)

$$x^2\omega'' + x\omega' + \left[x^2 - \left(l + \frac{1}{2}\right)^2\right]\omega = 0 \quad (17)$$

$v = \left(l + \frac{1}{2}\right)$, substitute equation (14)

$$x^2 y'' + xy' + (x^2 - v^2)y = 0 \quad (18)$$

$x_0 = 0$ is the first order pole of $p(x) = (1/x)$, the second order pole of $q(x) = \left(1 - v^2/x^2\right)$, so: $x_0 = 0$ is the regular singularity of the equation Determine the equation： $s(s-1) + s - v^2 = 0$

Determine the two roots of the equation:

$s_1 = v, s_2 = -v$;（$s_1 - s_2 = 2$ or v is an integer）

$$y(x) = a_0 x^S + a_1 x^{S+1} ... + a_K x^{S+K} ... (a_0 \neq 0)$$

The recursive formula for the coefficients is:

$$\left[(s+k)^2 - v^2\right]a_k + a_{k-2} = 0$$

among:

$$a_k = \frac{-a_{k-2}}{(s+k)^2 - v^2} = \frac{-a_{k-2}}{(s+k+v)(s+k-v) - v^2}$$

The general solution of the equation is:

$$y(x) = \sum_{k=0}^{\infty}\frac{(-1)^k}{\Gamma(v+k+1)}\left(\frac{x}{2}\right)^{v+2k} + \sum_{k=0}^{\infty}\frac{(-1)^k}{\Gamma(-v+k+1)}\left(\frac{x}{2}\right)^{-v+2k} \quad (19)$$

The calculation is in good agreement with the experimental results, which proves that our mathematical model is correct.

4 Conclusion

The 6H-SiC crystal was modeled by Materials Studio, and Al-doped with 6H-SiC. Then the 6H-SiC band diagram and density map were analyzed using the CASTEP module of Materials Studio. In order to facilitate the comparison, we compare the performance of other natural forms of SIC in the form of a table. The comparison items we used includeBreakdown electric field, Electron mobility, Hole mobility, Thermal conductivity and Electron saturation drift speed. The data of the comparison is shown in article. The following conclusions were obtained:

https://doi.org/10.1051/matecconf/201822701002

(1) 6H-SiC is a wide bandgap semiconductor material with a band gap of 2.2 eV, so it can be used as an LED luminescent material.

(2) 6H-Si has a variety of crystal forms, and the crystals of different forms have different forbidden bands. However, regardless of the crystal form, the forbidden band width is larger than that of common semiconductor materials such as silicon and germanium, so 6H-SiC is used as Semiconductor materials can reduce the leakage current of semiconductor devices, and 6H-SiC also has high temperature resistance, so it can replace semiconductor materials such as Si and Ge under high temperature conditions.

(3) Doping Al with 6H-SiC as a substrate can effectively change the nonlinear conductivity of 6H-SiC, which has a certain effect on improving semiconductor characteristics. In addition, the adsorption of metal impurities such as Ti, Fe, Ca, Mg on the surface of 6H-SiC can also effectively change the conductivity of 6H-SiC crystal.

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