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DENSITY OF STATES AND EFFECTIVE MASS OF HEAVY, LIGHT AND SPLIT-OFF HOLES NEAR THE VALENCE VAND EDGE OF SILICON

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ABSTRACT

The density of states and effective masses for the three types of subbands holes of silicon are investigated using the result of calculation for two energy band structures (DKK model and Kane model) with various band parameters obtained from the cyclotron experiments.

For DKK model the influences of the anisotropy in equi-energy surfaces are represented as modified coefficients. For Kane model those of the anisotropy and non-parabolicity in equi-energy surfaces are represented by modified functions. The limiting values of the density of states and effective masses at $E=0$ for heavy and light holes from Kane model coincide with those of DKK model and also for split-off holes. The influences of varying the values of band parameters are pronounced in the curvature of the density of states (or effective mass-ratio) and also found in the asymptotic values of three subbands holes.

§ 1. Introduction

The energy band structure near the valence band edge of silicon has been investigated using the $k \cdot p$ perturbation theory including the spin-orbit interaction. The valence band edge occurs at the center of the Brillouin zone ($k=0$), at which point a threefold orbital degeneracy is found if the spin-orbit interaction is not considered. The spin-orbit interaction partially removes the degeneracy by lowering the two bands with antiparallel spin with respect to the four bands with parallel spin. The former is known as split-off holes band and the latter as heavy and light holes band, respectively.

The split-off band has not so much been investigated because the probability of finding holes in that subbands is very small. But we can expect small contributions from the split-off holes to be found in transport properties of silicon. For example, in its drift mobility the split-off holes may contribute to the temperature dependence different from -3/2 power law even if we assume highly pure silicon crystals with parabolic valence bands.

It is important to obtain the density of states for the three subbands to estimate the properties of silicon. We use two model for the valence band and seven sets of band parameters which were measured and published previously [1], [5], [6] and [7]. One of the band structure model is based on Kittel et al. [1], called as DKK model in this paper. The other is called as Kane model which is based on Kane [2] and Asche *et al.* [3]. Using these two models and various values of band parameters we have obtained the density of states and the effective masses for three subbands holes.

From the resulting density of states we have obtained the formula of the density of states useful on future numerical works; for DKK model we introduced a modified coefficient which represents the slight anisotropy of equi-energy surfaces and for Kane model a modified function which represents the strong anisotropy and non-parabolicity.

2. Theory

The $E-k$ dispersion relation of DKK model proposed by Dresselhaus, Kip and Kittel [1] are given in spherical coordinates k, θ and ϕ as follows,

$$E=(-A\pm\sqrt{B^2+C^2\mu})k^2\,, \quad \text{for heavy } (-) \text{ and light } (+) \text{ holes,} \tag{1}$$

and

$$E=-Ak^2+\Delta\,, \tag{2}$$

with

$$\mu=\sin^2\theta(\sin^2\theta\cos^2\phi\sin^2\phi+\cos^2\theta)\,, \tag{3}$$

where A, B and C are band parameters which are determined from the cyclotron resonance constants, and are summarized in Table 1. Δ is the energy difference of $p_{3/2}$ and $p_{1/2}$ levels at $k=0$. m_0 is the free electron mass. Kittel *et al.* have obtained eqs. (1) and (2) assuming that the interaction between heavy, light and split-off holes can be neglected because those terms affect the roots only in the order k^4/Δ.

On the other hand, Kane solved complete 6×6 secular equation for energy eigenvalues, which is valid even in higher energy states than DKK model. According to Asche *et al.* [3], the secular equation of the valence band of silicon can be rewritten in cubic equation to k^2 in spherical coordinates as

$$ak^6+bk^4+ck^2+d=0\,, \tag{4}$$

with

$$a=-(A+2B)(A-B)^2+3(A-B)C^2\mu-(N-3B)^2(2N+3B)\nu\,,$$

$$b=3[(A^2-B^2)-C^2\mu](E'+\Delta/3)\,,$$

$$c=-3AE'(E'+2\Delta/3)\,,$$

$$d=E'^2(E'+\Delta)\,,$$

Table 1. Sets of band parameters used in calculation. The value of A is known with a considerably higher degree of accuracy than B and N. We chose four additional sets considering inaccuracies of the values of B and N. All values are represented in atomic unit ($\hbar=1$. $m_0=1/2$ and $e^2=2$).

SET	BAND PARAMETERS				REF.
	A	B	N	$\lvert C\rvert$	
I	−4.27	−0.63	−8.75	4.93	5,6
I-B$^-$	−4.27	−0.71	−8.75	4.90	8
I-B$^+$	−4.27	−0.55	−8.75	4.96	8
I-N$^-$	−4.27	−0.63	−9.00	5.08	8
I-N$^+$	−4.27	−0.63	−8.50	4.78	8
II	−4.22	−0.79	−8.61	4.78	7
III	−4.00	−1.10	−7.70	4.02	1

$C^2=\dfrac{N^2-9B^2}{3}$

$$\mu=\sin^2\theta(\sin^2\theta\cos^2\phi\sin^2\phi+\cos^2\theta),$$

$$\nu=\sin^4\theta\cos^2\theta\cos^2\phi\sin^2\phi,$$

and

$$C^2=(N^2-9B^2)/3,$$

where A, B, C and N are the same parameters as in eqs. (1) and (2). E' represents the hole energy taken from the top of the valence band edge negatively.

The solutions to eq. (4) which represent the $E-k$ dispersion relations near the valence band edge are given as,

$$k_H^2=-2\sqrt{\frac{-p}{3}}\cos(\alpha+\pi)-\frac{b}{3a}, \tag{5}$$

$$k_L^2=-2\sqrt{\frac{-p}{3}}\cos(\alpha+\pi/3)-\frac{b}{3a}, \tag{6}$$

and

$$k_S^2=-2\sqrt{\frac{-p}{3}}\cos(\alpha-\pi/3)-\frac{b}{3a}, \tag{7}$$

with

$$p=\frac{c}{a}-3\left(\frac{b}{3a}\right)^2,$$

$$q=\frac{d}{a}-\frac{c}{a}\left(\frac{b}{3a}\right)+2\left(\frac{b}{3a}\right)^3,$$

and

$$\alpha=\frac{1}{3}\cos^{-1}\left[-\frac{q}{2\sqrt{(-p/3)^3}}\right].$$

By using $i=H, L$ and S we distinguish three hole subbands known as heavy, light and split-off band, respectively.

As seen in eqs. (1) and (2), DKK model is parabolic but shows a slight anisotropy of the equi-energy surfaces. Kane band structure given by eqs. (5), (6) and (7) shows, however, non-parabolicity as well as anisotropy of equi-energy surfaces.

The density of states is defined as

$$g_{i(E)}=\frac{1}{4\pi^3}\int\frac{ds}{|\nabla_k E|}.$$

For DKK model, the following three solutions can be obtained;

$$g_H=\frac{1}{8\pi^3}\left(\frac{2m_0}{\hbar^2}\right)^{3/2}H\sqrt{E}\,, \tag{8}$$

$$g_L=\frac{1}{8\pi^3}\left(\frac{2m_0}{\hbar^2}\right)^{3/2}L\sqrt{E}\,, \tag{9}$$

and

$$g_S=\frac{1}{8\pi^3}\left(\frac{2m_0}{\hbar^2}\right)^{3/2}S\sqrt{E-\Delta}\,, \tag{10}$$

where $g_i(i=H, L$ and $S)$ means the density of states for each subbands holes, respectively. $I(=H, L$ and $S)$ is a modified coefficient which represents the anisotropy of DKK model and defined as,

$$H=\int\frac{d\Omega}{(-A-\sqrt{B^2+C^2\mu})^{3/2}}\,, \tag{11}$$

$$L=\int\frac{d\Omega}{(-A+\sqrt{B^2+C^2\mu})^{3/2}}\,, \tag{12}$$

and

$$S=\int\frac{d\Omega}{(-A)^{3/2}}. \tag{13}$$

In Table 2, those modified coefficients calculated for each band parameters are shown.

For Kane model, the $E-k$ dispersion relations are rewritten as

$$k_i^2=\frac{2m_0}{\hbar^2}u_i(E', \theta, \phi). \tag{14}$$

From eq. (14) the density of states for Kane model are given as

$$g_{i(E')}=\frac{1}{8\pi^3}\left(\frac{2m_0}{\hbar^2}\right)^{3/2}\int|\partial u_i/\partial E'|u_i^{1/2}d\Omega. \tag{15}$$

Table 2. Modified coefficients for DKK model calculated from eqs. (11), (12) and (13) using the values of band parameters in Table 1. All resulting values are also represented in atomic unit.

SET	Modified Coefficient for DKK		
	H	L	S
I	4.805	0.769	1.424
I-B^-	4.839	0.766	1.424
I-B^+	4.782	0.772	1.424
I-N^-	5.105	0.759	1.424
IN^+	4.537	0.780	1.424
II	4.921	0.778	1.450
III	4.964	0.847	1.571

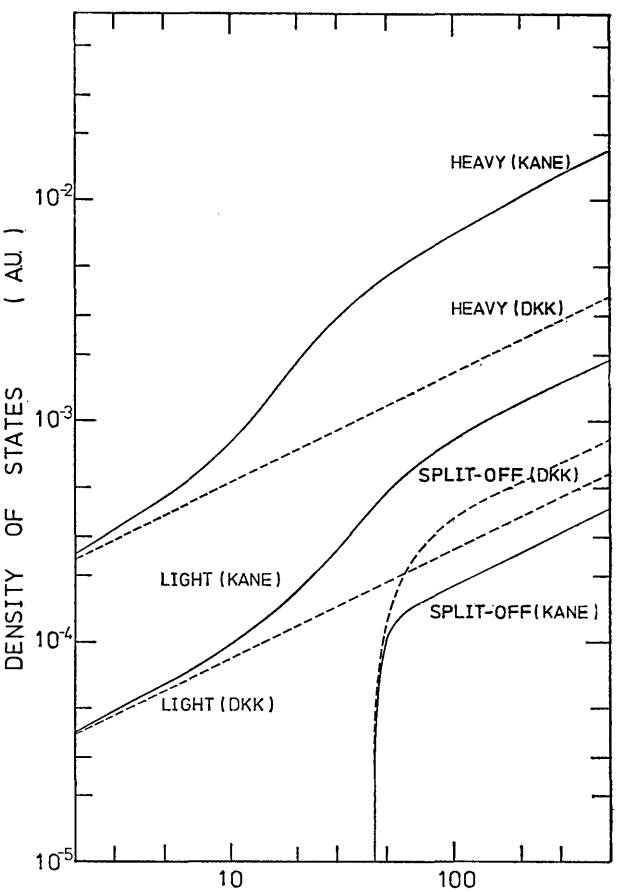

Fig. 1. Density of states for three subbands holes in the valence band of silicon calculated from DKK and Kane models. The values of density of states are represented in atomic unit.

The integration should be carried out on the equi-energy surface. The resulting density of states for each three subbands holes are shown in Fig. 1.

The effective mass is determined by comparing the density of states expressed by the effective mass with the density of states obtained for each model. For DKK model the effective mass are given for three subbands as

$$\frac{m_H}{m_0}=\left(\frac{H}{4\pi}\right)^{2/3}, \tag{16}$$

$$\frac{m_L}{m_0}=\left(\frac{L}{4\pi}\right)^{2/3}, \tag{17}$$

$$\frac{m_s}{m_0}=\left(\frac{S}{4\pi}\right)^{2/3}, \tag{18}$$

and for Kane model as

$$\frac{m_i}{m_0}=\left(\frac{\int u_i{}^{1/2}(E',\theta,\phi)u'_i(E',\theta,\phi)d\Omega}{4\pi\sqrt{E'}}\right)^{2/3}, \tag{19}$$

where

$$u_i'(E',\theta,\phi)=\frac{\partial}{\partial E'}u_i(E',\theta,\phi)\,. \tag{20}$$

The numerical calculation was carried out as follows; each equi-energy surface was divided in 1152 elements and the integration was performed by Simpson's method. The integration was found to converged when more than 648 elements were used.

3. Results and Discussion

The density of states calculated from DKK model agrees with those calculated from Kane model below several millielectron-volt. Since the equi-energy surfaces of both heavy and light holes for DKK model have the parabolicity between the energy and the magnitude of the wave vector, the energy dependence of the density of states for three subbands holes obeys $E^{1/2}$ law like free carriers. The difference between DKK model and free carrier model arises from the anisotropy of the equi-energy surfaces and is represented by the modified coefficients defined in eqs. (11), (12) and (13).

According to Kane model, the $E^{1/2}$ dependence of the density of states breaks down at several tens of millielectron-volt for both heavy and light holes. Above about 100 meV, however, the $E^{1/2}$ dependence is found to be restored. Those complicated energy dependence of the density of states for heavy and light holes are produced by the interactions between subbands when the split-off holes band appears above the split-off energy.

It is very important to estimate the magnitude of the density of states near the band edge in order to interpret electrical or optical properties of semiconductors.

The density of states calculated from Kane model involves the anisotropy and non-parabolicity of equi-energy surfaces near the valence band edge. We tried to construct an approximate formula to describe the density of states for heavy and light holes near the valence band edge because heavy and light holes affect most of electrical and optical properties except at very high temperature. We calculated the deviation of the density of states between Kane and DKK model, which are represented by using the following modified form of the constant C, which is a function of E,

$$C_{(E)}=\frac{\omega(\log E-\zeta)}{\sqrt{\chi+(\log E-\zeta)^2}}+\xi\,. \tag{21}$$

The function reproduces the non-parabolicity and strong anisotropy of equi-

Table 3. Adjustable parameters of a modified function for heavy and light holes by using band parameters "set I". In calculation, energy is taken in millielectronvolt.

HOLE	ζ	ξ	χ	ω
HEAVY	1.354	2.725	0.162	1.725
LIGHT	1.582	2.150	0.110	1.150

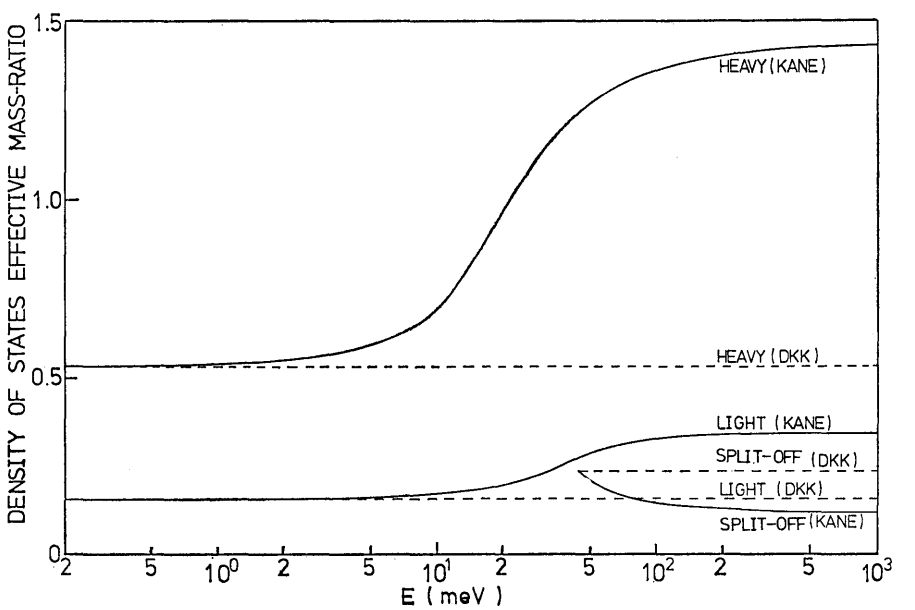

Fig. 2. Energy dependence of the effective mass-ratios for three subbands holes of the valence band of silicon calculated from DKK and Kane models for set I.

energy surfaces. Values of adjustable parameters ζ, ξ, χ and w depend on band parameters. Therefore the formula of density of states useful near the valence band edge for heavy and light holes are given as

$$g_{i(E)} = \frac{1}{8\pi^3}\left(\frac{2m_0}{\hbar^2}\right)^{3/2}\sqrt{E}\, I\cdot\left[\frac{\omega(\log E-\zeta)}{\sqrt{\chi+(\log E-\zeta)^2}}+\xi\right], \tag{22}$$

where i ($=H$ or L) specifies the density of states for heavy and light holes band, respectively. I ($=H$ or L) is the modified coefficient defined in eqs. (11) or (12).

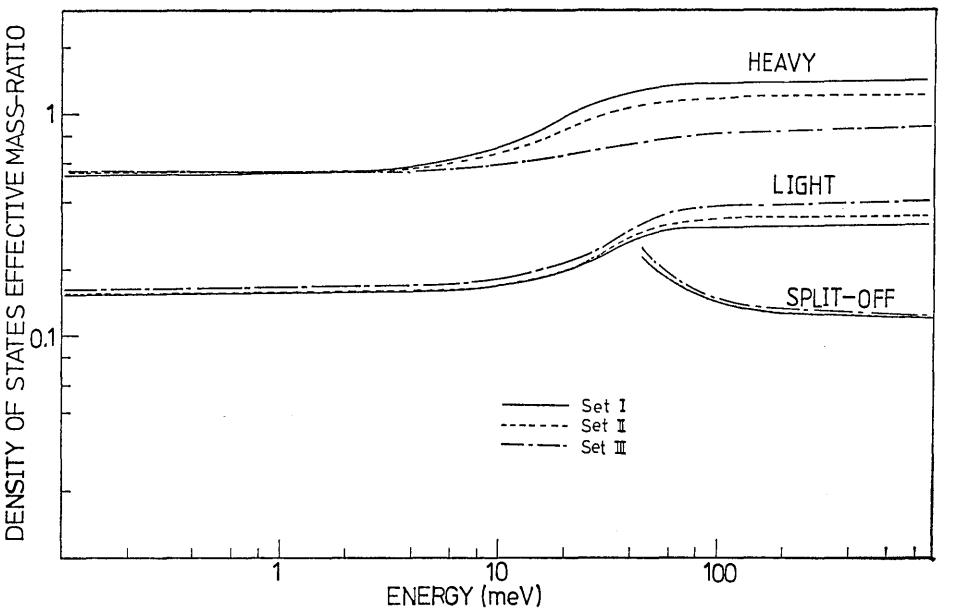

Fig. 3. Influence of varying band parameters in effective mass-ratios.

Table 4. Effective mass-ratio for three subbands calculated from DKK and Kane models with various band parameters.

SET	HEAVY			LIGHT			SPLIT-OFF		
	DKK	KANE		DKK	KANE		DKK	KANE	
	arbitrary energy	0.001 meV	1 eV	arbitrary energy	0.001 meV	1 eV	arbitrary energy	44.001 meV	1 eV
I	0.527	0.527	1.433	0.155	0.155	0.342	0.234	0.234	0.121
I-B$^-$	0.529	0.529	1.332	0.155	0.155	0.348	0.234	0.234	0.120
I-B$^+$	0.525	0.526	1.563	0.156	0.156	0.336	0.234	0.234	0.121
I-N$^-$	0.549	0.549	2.098	0.154	0.154	0.346	0.234	0.234	0.119
I-N$^+$	0.507	0.508	1.152	0.157	0.157	0.338	0.234	0.234	0.122
II	0.535	0.535	1.220	0.156	0.156	0.358	0.237	0.237	0.121
III	0.541	0.541	0.844	0.165	0.165	0.403	0.250	0.249	0.126

The values of adjustable parameters ζ, ξ, χ and w are shown in Table 3 for set I. Eq. (22) can be used for discussing the electrical or optical properties of semiconductors.

The effective masses are shown in Fig. 2 and 3. We can also recognize that the effective masses calculated from Kane model coincide with those from DKK model below 1 meV and our calculated effective mass of heavy holes shows a good agreement with the recent work [9]. The effective masses for both heavy and light holes increases with energy. For the split-off holes, however, it decreases with energy. The asymptotic values of the effective masses for light holes ($E=0$) is smaller than the one of the split-off holes ($E=\Delta$). But above 100 meV the effective mass of light holes becomes greater than the one of the split-off holes.

The influence of varying the values of the band parameters is pronounced in the curvature of the density of states (and effective mass-ratio) at about several tens of millielectronvolt and is found on the asymptotic values of three subbands holes, which are summarized in Table 4. It is found that the non-parabolicity and the strong anisotropy of three subbands and also the interaction with the split-off holes makes the energy dependence of the density of states complicated and thus makes the effective masses depend on the hole energy.

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