Quantization of the free charge carriers on InSb at room temperature

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Abstract

A new method of self-consistent quantum calculation of the density of the space charge near the surface of a crystal is carried out for the semiconductor with nonparabolic (Kane) dispersion law of bands. The remarkable feature is the solution of the Schrödinger equation for electrons and holes in the energy range, including both bound energy states and states in the continuum. Theoretical voltage-capacitance dependence is calculated and coincides with experimental data. The dependence of the electron mass and surface mobility from the value of surface potential are analyzed.

Keywords: InSb, self-consistent quantum calculation, voltage-capacitance, effective mass, surface mobility.

1 Method of self-consistent quantum calculation

When an electric field is applied perpendicularly to the surface of the semiconductor, the space charge region (SCR) is induced in the subsurface layer [1]. In frames of the one-particle Hartree approximation the distribution of charge density is defined from self-consistent solution of Poisson and Schrödinger equations [2]. In InSb at room temperature it is necessary to take into account simultaneously both type of charge carriers in the whole allowed range of energies. Therefore the calculation is based on the model of “semi-infinite crystal with a second fictitious border” [3] with modifications implied a specific character of Kane semiconductors.

The bulk dispersion law of Kane semiconductors is described by formula [4]

\[ k^2(E) = \frac{1}{P^2} \frac{(E - E_0)(E - E_0 + E_g)(E - E_0 + E_g + \Delta)}{(E - E_0 + E_g + \frac{2}{3}\Delta)}, \]  

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where $\mathbf{k}$ is wave vector, $P$ is the matrix element, accounting the interaction between the conductance and valence bands, $E_0 = \hbar^2 k^2 / (2m_0)$ is the energy of free electron with mass $m_0$, $E_g$ is the energy gap of semiconductor, $\Delta$ is the energy of spin-orbital splitting of valence band.

In general case the density of charge carriers in the bulk of semiconductor is determined by Fermi-Dirac statistic

$$\rho = \frac{2}{(2\pi)^3} \int f_0(k) \, dk,$$

where

$$f_0(k) = \frac{1}{1 + \exp[(E(k) - E_F)/(k_0T)].}$$

$E_F$ is the Fermi level energy; $k_0$ is the Boltzmann constant; $T$ is the absolute temperature.

Consider the crystal with the bounded coordinate $z \in [0, L^*]$ and the infinite coordinates $x, y \in ]-\infty, +\infty[. \text{ In frames of the one-particle Hartree approximation the wave function may be presented by } e^{i\mathbf{k} \cdot \mathbf{r}} \varphi_i(z, k_i), \text{ where } \varphi_i(z, k_i) \text{ is the enveloping wave function for the bounded state } E_i(k_i). \text{ Here are } k_i^2 = k_z^2 + k_x^2, k_x, k_y \in ]-\infty, +\infty[; r_i^2 = x^2 + y^2. \text{ After the change of variables } \varepsilon_i = \hbar^2 k_i^2 / (2m_n k_0 T), \varepsilon_i = E_i / (k_0 T), \varepsilon_g = E_g / (k_0 T) \text{ the concentrations of the electrons and hard holes can be found from expressions}

$$\rho_e(z) = \frac{m_n k_0 T}{\pi \hbar^2} \int_{0}^{+\infty} d\varepsilon_i \sum_{i} \frac{|\varphi_i(z, \varepsilon_i)|^2}{1 + \exp(\varepsilon_i - \varepsilon_F)}, \quad (3)$$

$$\rho_{hh}(z) = \sum_{j=1}^{+\infty} \Gamma_j(\varepsilon_j)|\varphi_j(z)|^2, \quad (4)$$

where

$$\Gamma_j(\varepsilon_j) = \frac{m_n k_0 T}{\pi \hbar^2} \ln(1 + \exp(-\varepsilon_j - \varepsilon_g - \varepsilon_F)).$$

Electrostatical potential into the SCR $V(z)$ created by external electric field satisfies the Poisson equation

$$\frac{d^2 V(z)}{dz^2} = q \left( \rho_e(z) - \rho_{hh}(z) + N_d - N_a \right) / \varepsilon_s + \varepsilon_{sc}, \quad V(0) = V_s; \quad V(L^*) = V_0(L^*). \quad (5)$$

Here $\varepsilon_{sc}$ is the static dielectric constant of the semiconductor; $N_d$ and $N_a$ are the concentrations of ionized donor and acceptor impurities, respectively.

In terms of quantum description in the one-particle Hartree approximation the wave functions $\varphi_i(z, k_i), \varphi_j(z)$ and eigenvalues $E_i(k_i), E_j$ of the free charge carriers are derived from solving of the equations

$$- \frac{\partial^2 \varphi_i(z, k_i)}{\partial z^2} = [k_i^2(E - V(z)) - k_i^2] \varphi_i(z, k_i) \quad (6)$$

$$\left( \frac{\hbar^2}{2m_n k_i} \frac{d^2}{dz^2} - qV(z) \right) \varphi_j(z) = E_j \varphi_j(z), \quad (7)$$

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Boundary conditions and normalization of all wave functions take the form

\[ \varphi(0) = \varphi(L^*) = 0; \int_0^{L^*} |\varphi(z)|^2 \, dz = 1. \]

The densities of charge carriers are calculated according to Eqs. (3) and (4). In our case at room temperature the integration is performed in the interval \( \varepsilon_\parallel \in [0,16] \) taking into account all quantum subbands up to \( \varepsilon_i(k_\parallel = 0) < 12 \) and \( | - \varepsilon_i - \varepsilon_g| < 12 \) for electrons and holes respectively. The self-consistent calculation of SCR is carried out in frames of the iteration scheme [3].

2 Experimental results and discussion

The following constants of the material [5] were used for calculations: \( \varepsilon_{sc} = 17.9; \; m_0 = 9.1 \cdot 10^{-31} \text{kg;} \; m_n = 0.013m_0; \; m_{hh} = 0.5m_0; \; N_{a,d} = 0; \; E_g = 0.165 - 2.8 \cdot 10^{-4}(T - 300) \text{eV;} \; T = 290 \text{K.} \) The voltage-capacitance dependence is an important measurable characteristics. The differential capacitance of SCR is given by

\[ C_{sc}(V_s) = \frac{dQ}{dV_s}, \quad \text{where} \quad Q = q \cdot \int_0^\infty [\rho_e(z) - \rho_{hh}(z) + N_a - N_d] \, dz. \]
The comparison between experimental data [6] and theoretical quantum calculation for InSb at room temperature is shown on Fig. 1. Good agreement of the experiment and quantum calculation in wide range of surface potentials demonstrates the efficiency of proposed mathematical model.

This model of calculation allows to carry out the detailed analysis of the change of the electron mass in SCR for the Kane semiconductor. The mass of electron in longitude direction is described by formula

$$\frac{1}{m_i(E_\parallel)} = \frac{1}{\hbar^2 k_i} \frac{dE_i}{dk_\parallel} = \frac{1}{m_n} \frac{dE_\parallel}{dE_i}.$$  

Determine the mean value of the electron mass $\overline{m}(z)$ as

$$\overline{m}(z) = \frac{\int_0^\infty m_i(\varepsilon_\parallel) \rho_e(z, \varepsilon_\parallel)^2}{\int_0^\infty \rho_e(z, \varepsilon_\parallel)^2} \frac{d\varepsilon_\parallel}{1 + \exp(\varepsilon_i - \varepsilon_F)}$$

One can see from Fig. 2a that near the surface the concentration of the “hard” electron is greater than in the bulk.

On the Fig. 2b is shown the average mass of electrons on $i$ energy level

$$\overline{m}_i = \frac{\int_0^\infty m_i(\varepsilon_i) d\varepsilon_i}{\int_0^\infty \int_0^\infty \frac{d\varepsilon_\parallel}{1 + \exp(\varepsilon_i - \varepsilon_F)}}.$$  

Let us introduce the mean mass of electron in SCR as

$$m_{SCR}(V_s) = \int_0^{2L_D} \overline{m}(z) \rho_e(z) dz$$

where $L_D$ is the length of Debye.
This dependence is shown on Fig. 3a. It is obvious that the mean mass of electron increases monotonically with growth of surface potential. This regularity must arise also in transport phenomena in subsurface layer of Kane semiconductor.

Indeed, let us write the expression of the electron mobility in the bulk of the semiconductor and in SCR by $m_{SCR}(V_s)$:

$$
\mu_b = \frac{q \tau_b}{m_{SCR}(V_s = 0)}, \quad \mu_s = \frac{q \tau_s}{m_{SCR}(V_s)}.
$$

Assume that there is no additional mechanisms of scattering on the surface other than the ones in the bulk ($\tau_s = \tau_b$). Then we have

$$
\mu_s(V_s) = \frac{\mu_b m_{SCR}(V_s = 0)}{m_{SCR}(V_s)}.
$$

The dependence of surface mobility on $N_s = \int_0^{L^*} (\rho_e(z) - \rho_{hh}(z) + N_a - N_d) \, dz$ is shown on Fig. 3b, where $\mu_b = 7.8 \, m^2/(V \cdot s)$ [5]. As one can see from Fig. 3b, for InSb at room temperature the surface mobility, even in absence of additional mechanisms of surface scattering (interaction with phonon, roughnesses, etc [1]) decreases monotonically with growth of the surface potential. This effect is stipulated by nonparabolic dispersion law of conductance band, which leads to the dependence of electron mass on energy and surface potential.

The results can be very useful for studying of mobility of electrons and holes in the accumulation and inversion layers on the surface of the Kane semiconductors.

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