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1 月 15 日汇报-Semiconductor Equation 物理模型的建立

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初版 Gummel 迭代的 Semiconductor Equation 的物理模型建立如下 [1]:

$$\begin{cases} -\frac{\varepsilon}{q}\Delta\psi + n - p + C = 0 \\ \nabla\cdot\mathbf{J}_n - qR = 0, \mathbf{J}_n = -q\mu_n n\nabla\phi_n \\ \nabla\cdot\mathbf{J}_p + qR = 0, \mathbf{J}_p = -q\mu_p p\nabla\phi_p \end{cases} \Rightarrow \begin{cases} f_1 : -\frac{\varepsilon}{q}\Delta\psi + n - p + C = 0, \\ f_2 : \nabla\cdot[-q\mu_n n\nabla\phi_n] - qR = 0, \\ f_3 : \nabla\cdot[-q\mu_p p\nabla\phi_p] + qR = 0. \end{cases} \tag{1.1}$$

其中[1][2]。

$\mathbf{J}_n = \mu_n n\nabla E_{F_n} = -q\mu_n n\nabla\phi_n$	$\mathbf{J}_p = \mu_p p\nabla E_{F_p} = -q\mu_n n\nabla\phi_p$
$E_{F_n}(\phi_n) = -q\phi_n$	$E_{F_p}(\phi_p) = -q\phi_p$
$n = g_n(E_{F_n}(\phi_n), E_c'(\psi))$	$p = g_p(E_{F_p}(\phi_p), E_c'(\psi))$
$g_n(E_{F_n}, E_c') = N_c \exp(\frac{E_{F_n}-E_c'}{k_b T})$	$g_p(E_{F_p}, E_v') = N_v \exp(\frac{E_v'-E_{F_p}}{k_b T})$
$R = U - G$	$C = N_A^- - N_D^+ - \frac{\rho_s}{q}$

[1] 载流子浓度的计算采用的是波尔兹曼分布。

[2] 迭代的自变量取 ϕ_n, ϕ_p 还是 n, p?

《AN APPROXIMATE NEWTON METHOD FOR THE SOLUTION OF ···》

设边界条件 $\partial\Omega$ 包括了 Dirichlet 和 Neumann 边界条件：

$$
\begin{aligned}
\psi(x) &= \psi_D(x), x \in \partial\Omega_D, \\
\phi_n(x) &= \phi_{n_D}(x), x \in \partial\Omega_D, \\
\phi_p(x) &= \phi_{p_D}(x), x \in \partial\Omega_D, \\
\nabla\psi \cdot \nu = \mathbf{J}_n \cdot \nu &= \mathbf{J}_n \cdot \nu = 0, x \in \partial\Omega_N.
\end{aligned}
$$

其中，$\partial\Omega = \partial\Omega_D \cup \partial\Omega_N$, $\partial\Omega_D \cap \partial\Omega_N = \oslash$[1].

n：电子载流子浓度	p：空穴载流子浓度
E_{F_n}：电子准费米势能级	E_{F_p}：空穴准费米势能级
J_n：电子电流密度	J_p：空穴电流密度
U：载流子复合项	R：载流子生成项
ϕ_n：电子准费米势	ϕ_p：空穴准费米势

《A physics-based strategy for choosing initial iterate for solving drift-diffusion equations》

假设 Ω 区域的边界包含 Dirichlet Boundary Condition 和 Neumann Boundary Condition： $\partial\Omega = \Gamma_D \cup \Gamma_N$. 则边界条件如下 [2]：

$$\begin{cases} \psi = \psi_{bc}, n = n_{bc}, p = p_{bc}, & on\ \Gamma_D, \\ \frac{\partial \psi}{\partial n} = 0, J_n \cdot n = 0, J_p \cdot n = 0, & on\ \Gamma_N. \end{cases} \tag{1.2}$$

依据半导体材料性质，Ω 可以分为 N 型区域（N-type）（$N_D - N_A \geqslant 0$）和 P 型区域（P-type）（$N_D - N_A \leqslant 0$）： $\Omega = \Omega_N \cup \Omega_P$.

$$\Omega^N = \bigcup_{i=1}^{K} \Omega_i^N, \quad \Omega^P = \bigcup_{j=1}^{L} \Omega_j^P.$$

假设对边界表明施加了偏置电压（bias voltage）V_{app}，施加的区域为 $\Gamma_v \subset \Gamma_D$：

- 若 $\Gamma_v \cap \partial\Omega_i^N \neq \emptyset$，则在 N 型区域 Ω_i^N 边界上存在接触电压（contact voltage）。
- 若 $\Gamma_v \cap \partial\Omega_j^P \neq \emptyset$，则在 P 型区域 Ω_j^P 边界上存在接触电压（contact voltage）。

定义函数：

$$\xi(x) = \begin{cases} V_{app}, & x \in \Gamma_v, \\ 0, & x \in \Gamma_D \backslash \Gamma_v. \end{cases} \tag{1.3}$$

则欧姆接触边界条件（ohmic contact boundary condition）如下 [2]：

$$n_{\mathrm{bc}} = \frac{N_D - N_A + \sqrt{(N_D - N_A)^2 + 4{n_{\mathrm{ie}}}^2}}{2},$$

$$p_{\mathrm{bc}} = \frac{N_A - N_D + \sqrt{(N_D - N_A)^2 + 4{n_{\mathrm{ie}}}^2}}{2},$$

$$\psi_{\mathrm{bc}} = \frac{k_b T}{q} \mathrm{a}\sinh\left((N_D - N_A)/(2n_{\mathrm{ie}})\right) + \xi.$$

- 对于 n 型区域 [3, 4]:

$$n_{\mathrm{bc}} = \frac{N_D + \sqrt{(N_D)^2 + 4{n_{ie}}^2}}{2}, p = \frac{n_{ie}^2}{n}$$
$$\psi = \psi_t \ln\left(\frac{N_D}{n_{ie}}\right) + V_{app}$$

- 对于 p 型区域:

$$p_{\mathrm{bc}} = \frac{N_A + \sqrt{(N_A)^2 + 4{n_{ie}}^2}}{2}, n = \frac{n_{ie}^2}{p}$$
$$\psi = -\psi_t \ln\left(\frac{N_A}{n_{ie}}\right) + V_{app}.$$

设边界 $\partial\Omega$ 由两部分组成:

1. $\partial\Omega_p$ represents those parts of the boundary which correspond to real "physical" boundaries like contacts and interfaces to insulating material.
   - $\partial\Omega_p$ can be roughly split into three classes:

$$\partial\Omega_p = \partial\Omega_O \cup \partial\Omega_S \cup \partial\Omega_I.$$

   - $\partial\Omega_O$: ohmic contacts
   - $\partial\Omega_S$: Schottky contacts
   - $\partial\Omega_I$: interfaces to insulating material
2. $\partial\Omega_A$ consists of artificial boundaries which have to be introduced, for instance, to separate neighboring devices in integrated circuits.

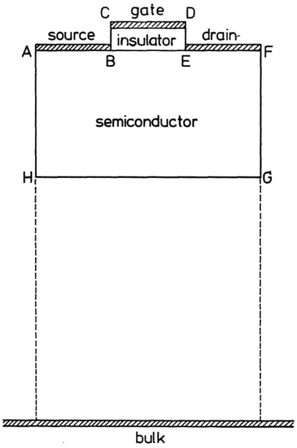

图: Simulation geometry of a planar MOSFET

- General form:

$$g\left(\psi, \frac{\partial \psi}{\partial t}, I, \frac{\partial I}{\partial t},\right) = 0$$

where $I = \int_{\partial D_O} (\mathbf{J}_n + \mathbf{J}_p) \cdot \mathrm{d}\mathbf{A}$ is the total current density

- Voltage controlled:

$$\psi(t) - \psi_b - \psi_D(t) = 0$$

where ψ_b is the built-in potential and $\psi_D(t)$ is the externally applied bias.

- Current controlled:

$$\int_{\partial D_O} (\mathbf{J}_n + \mathbf{J}_p) \cdot \mathrm{d}\mathbf{A} - I_D(t) = 0$$

- 假设欧姆接触是理想的导电性，这意味着在边界中没有电压下降：

$$\psi(t) - \psi_b = \text{const}$$

- 假设热平衡（对应于无限的表面复合速度）和空间电荷消失：

$$\begin{cases} np - n_{ie}^2 = 0 \\ n - p - C = 0 \end{cases} \Longrightarrow \begin{cases} n = \dfrac{\sqrt{C^2 + 4n_{ie}^2} + C}{2} \\ p = \dfrac{\sqrt{C^2 + 4n_{ie}^2} - C}{2} \end{cases}$$

其中 $C = N_D - N_A$.

1. For the electrostatic potential in the case of a voltage drive: (对于电压驱动情况下的静电势)

$$\psi(t) - \psi_b + \psi_s - \psi_D(t) = 0, \tag{2.1}$$

   - $\psi_D(t)$ denotes the externally applied bias,
   - ψ_b is the built-in potential,
   - ψ_s represents the Schottky barrier height, which is a characteristic quantity of the metal and the semiconductor with which the Schottky contact is fabricated.

2. Concerning the interplay of the thermionic emission and diffusion theories:

$$\vec{J}_n \cdot \vec{n} = -q \cdot v_n \cdot \left[n - \frac{\left(\sqrt{C^2 + 4 \cdot n_{ie}^2} + C\right)}{2} \right], \vec{J}_p \cdot \vec{n} = q \cdot v_p \cdot \left[p - \frac{\left(\sqrt{C^2 + 4 \cdot n_{ie}^2} - C\right)}{2} \right].$$

v_n, v_p denote the thermionic recombination velocities for electrons and holes.

Assume that no current at all flows through the Schottky contact:

$$\begin{cases} v_n = 0 \\ v_p = 0 \end{cases} \Rightarrow \begin{cases} \vec{J}_n \cdot \vec{n} = 0 \\ \vec{J}_p \cdot \vec{n} = 0 \end{cases}$$

This assumption is at first glance reasonable since for most of the practical operating conditions the Schottky contact operates in the reverse biased mode, where the current flow is indeed relatively small.

在大多数实际操作条件下，肖特基接触处于反向偏置模式，其中电流流动确实相对较小。

Interfaces to insulating material

对于静电势 ψ:

- Obey the law of GauB in differential form:

$$\varepsilon_{sem} \cdot \left.\frac{\partial \psi}{\partial \vec{n}}\right|_{sem} - \varepsilon_{ins} \cdot \left.\frac{\partial \psi}{\partial \vec{n}}\right|_{ins} = Q_{int}.$$

  * ε_{sem} and ε_{ins} denote the permittivity in the semiconductor and the insulator, respectively.
  * Q_{int} represents charges at the interface.

- Assume in the insulator a vanishing electric field component perpendicular to the interface:

$$\varepsilon_{sem} \cdot \left.\frac{\partial \psi}{\partial \vec{n}}\right|_{sem} = Q_{int}.$$

- Quite often the existence of interface charges is also neglected:

$$\partial \psi / \partial \vec{n} = 0.$$

For the continuity equations the current components perpendicular to the interface must equal the surface recombination rate R^{SURF}:

$$\begin{cases} \vec{J}_n \cdot \vec{n} = -q \cdot R^{SURF}, \\ \vec{J}_p \cdot \vec{n} = q \cdot R^{SURF}. \end{cases}$$

Assume that surface recombination disappears:

$$\begin{cases} \vec{J}_n \cdot \vec{n} = 0 \\ \vec{J}_p \cdot \vec{n} = 0 \end{cases}$$

This type of boundary is not based on physical consideration. Therefore, it is called an artificial boundary.

$$\frac{\partial \psi}{\partial \vec{n}} = 0, \tag{2.2}$$

$$\frac{\partial n}{\partial \vec{n}} = 0, \tag{2.3}$$

$$\frac{\partial p}{\partial \vec{n}} = 0. \tag{2.4}$$

Disadvantage:

- A-B 和 E-F 的距离必须足够大，以使 A-H 和 F-G 处的人工边界条件引入的误差小到可以忍受。

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