Mid-term exam, VLSI Devices, Spring semester, 2024

April 15, 2024

Clearly distinguish vectors and scalars.

1. Consider a body-centered cubic crystal system. Three basis vectors of the direct lattice are:

$$\mathbf{a}_1 = \frac{a}{2}(-\mathbf{x} + \mathbf{y} + \mathbf{z})$$

$$\mathbf{a}_2 = \frac{a}{2}(\mathbf{x} - \mathbf{y} + \mathbf{z})$$

$$\mathbf{a}_3 = \frac{a}{2}(\mathbf{x} + \mathbf{y} - \mathbf{z})$$

In the above expressions, a is a lattice constant. Also, $\mathbf{x},$ $\mathbf{y}$, and $\mathbf{z}$ are unit vectors.

The reciprocal lattice vectors are defined as follows:

$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

$$\mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

$$\mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

(1) Calculate the volume of the primitive cell, $\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)$.

(2) Calculate the reciprocal lattice vectors, $\mathbf{b}_1$, $\mathbf{b}_2$, and $\mathbf{b}_3$.

(3) Using the calculated reciprocal lattice vector, calculate $\mathbf{a}_i \cdot \mathbf{b}_j$. In this case, i and j can be 1, 2, or 3.

2. The Bloch theorem states that under a periodic potential the wavefunction can be expressed in a form of

$$\psi(\mathbf{r}) = u(\mathbf{r}) \exp(i\mathbf{k} \cdot \mathbf{r})$$

In the above expression, i is the imaginary unit. The function, $u(\mathbf{r})$, is periodic within the direct lattice.

$$u(\mathbf{r} + \mathbf{R}) = u(\mathbf{r})$$

In the above expression, $\mathbf{R}$ is a lattice vector.

(1) Calculate the Laplacian of $\psi(\mathbf{r})$. Note that the Laplacian of fg is $f\nabla^2 g + 2\nabla f \cdot \nabla g + g\nabla^2 f$ for two scalar functions, f and g.

(2) The wavefunction must satisfy the Schrödinger equation:

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

In the above expression, $V(\mathbf{r})$ is the potential energy and E is the energy. From the Bloch wavefunction and the answer of (1), derive an equation for $u(\mathbf{r})$.

3. Consider the following E-$\mathbf{k}$ relation:

$$E(\mathbf{k}) = \frac{\hbar^2}{2m_0}\left[Ak^2 - \sqrt{B^2k^2 + C^2\left(k_x^2k_y^2 + k_y^2k_z^2 + k_z^2k_x^2\right)}\right]$$

In the above expression, A, B, and C are constants. Also, k^2 is $k_x^2 + k_y^2 + k_z^2$.

(1) Calculate the x-directional component of the group velocity, $v_x = \frac{1}{\hbar}\frac{\partial}{\partial k_x}E(\mathbf{k})$.

(2) Calculate the xx component of the inverse mass tensor, $m_{xx}^{-1} = \frac{1}{\hbar^2}\frac{\partial^2}{\partial k_x^2}E(\mathbf{k})$.

4. In our lectures, we had a long discussion on the carrier densities. Under some reasonable approximations, simple but important relations for the carrier densities have been derived.

(1) Express n in terms of n_i (intrinsic carrier density), ϕ (electrostatic potential), and ϕ_n (electron quasi-Fermi potential).

(2) Express p in terms of n_i, ϕ, and ϕ_p (hole quasi-Fermi potential).

(3) At equilibrium, we may assume $\phi_n = \phi_p = 0$. Consider a sample whose ionized donor are acceptor densities are N_d^+ and N_a^-, respectively. By using the answers of (1) and (2) and the charge neutrality, calculate the electrostatic potential.

5. The Poisson equation must be considered in the semiconductor device:

$$\nabla \cdot (-\epsilon \nabla \phi) = \rho$$

We can consider two different boundary types. For each type, describe an appropriate boundary condition.

(1) Ideal Ohmic contact (Metal / highly-doped semiconductor)

(2) Non-contact boundary

6. The electron current density is given as

$$\mathbf{J}_n = -q\mu_n n \nabla \phi + qD_n \nabla n$$

By using the Einstein relation and the answer of Problem 4.(1), derive an alternative expression for $\mathbf{J}_n$. The intrinsic carrier density, n_i, is constant.

7. The SRH recombination rate is given as

$$R_n - G_n = R_p - G_p = \frac{np - n_i^2}{\tau_p(n + n_1) + \tau_n(p + p_1)}$$

In the above expression, n_1 and p_1 are given numbers. They are usually small, $n_1 \approx n_i$ and $p_1 \approx n_i$. Show that the recombination rate is determined by the excessive minority carrier density. For example, the excessive hole density in the n-type sample determines the recombination rate.

8. In the drift-diffusion model, the following three equations must be solved:

$$\nabla \cdot \mathbf{D} = q(p - n + N_d^+ - N_a^-)$$

$$\frac{\partial}{\partial t} n = \frac{1}{q} \nabla \cdot \mathbf{J}_n + G_n - R_n$$

$$\frac{\partial}{\partial t} p = -\frac{1}{q} \nabla \cdot \mathbf{J}_p + G_p - R_p$$

Using the three equations, calculate $\nabla \cdot \left(\mathbf{J}_n + \mathbf{J}_p + \frac{\partial}{\partial t} \mathbf{D} \right)$.