Transport Properties of “Man-Made” Crystalline Semiconductor Superlattices

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Abstract: The electron transport in semiconductor superlattices exhibits interesting phenomena which are quite different from those that occurred in a bulk material. This depends on the electronic band structures in the semiconductor superlattices. The energy band gaps of the superlattices are aligned, but the magnitudes of the band gaps are different. The difference in the width of the energy gap in different semiconductors forms the boundary of the conductivity band for perfect semiconductor superlattices that is modulated periodically and leads to the formation of energy minibands.

Key words: Semiconductor superlattices, band theory, bloch theorem, schrödinger equation, kronig-penney model.

1. Introduction

Innovations in technology are improving all the time with exciting new techniques emerging relevant to almost all areas that make use of ultrafast electrons. Electrons in semiconductor superlattices, an example of periodic crystal, exhibit wide range of nonlinear effects that are useful for application in these ultrafast electronics. This is due to the arrangement or the structure of the semiconductor superlattices that are formed by a number of periodic layers. Semiconductor superlattices are a single-crystal structure, and its chemical composition varies periodically in space at distances (1-10 nm), which is greater than the periods of its constituent materials. It is a man-made structure that can be made to investigate a fundamental quantum mechanical phenomenon, which forms quantised energy states [1], since the thickness of the layers, the number of periods and periodic potential strength can be controlled [2]. The motion of electrons in the superlattices is modified by the atoms arrangement in a periodic way if it is assumed that there is no interaction between the electrons. These man-made superlattices serve as a periodic potential

for conduction electrons, since electron dynamics cannot occur in natural superlattices because its formation is not well understood and is difficult to control. These nanostructures are formed from several alternating layers of different semiconductor materials [3]. The arrangement of An Aluminum Arsenide and Gallium Arsenide (AlAs / GaAs) superlattice example is shown.

2. Theory

Band theory is used to understand the dynamics of particles in the crystal. The energy bands in solids are the fundamental electronic structure of a crystal. Consider the electron behaviour in a one-dimensional periodic lattice that can be explained by the Schrodinger equation. For a particle with energy E that is moving in the periodic potential $V(x)$, the crystal lattice will have an eigenstate, the crystal lattice will have an eigenstate $\psi(x)$ that satisfies Eq. (1):

$$\hat{H}\psi = \left(-\frac{\hbar^2}{2m} \nabla^2 + V(x) \right) \psi(x) = E\psi(x) \quad (1)$$

The Bloch theorem states that the eigen-functions of the wave equation for a periodic potential are the product of a plane wave $\exp(ikx)$ and a wave function $u_k(x)$ with periodicity of the crystal lattice

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[4]. Therefore, the eigenstate can be written as Eq. (2):

$$\psi_k(x) = u_k(x) \exp(ikx) \quad (2)$$

where $u_k(x)$ is aperiodic function, and also the translational symmetry of the lattice. A periodic potential $V(x)$ will create a spatial lattice generated by the atoms in a solid or by counter propagating lasers in an optical lattice [5]. The Bloch wave functions for a particular system can be determined by solving Schrödinger's equation, where E is the energy of the system and ψ is the wave function as Eq. (3):

$$\hat{H}\psi = E\psi \quad (3)$$

where the Hamiltonian operator $\hat{H}$ of a periodic system of infinite extent that is a large periodic potential is

$$\hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + V(x) \quad (4)$$

where $V(x)$ is the potential energy of the system and has the periodicity of the lattice, m is the mass of the quantum particles and ∇^2 is the Laplacian [6, 7]. In Eq. (4), $\hbar = h/2\pi$ where $h = 1.054 \times 10^{-34} \text{Js}^{-1}$, the Planck constant [8, 9]. Eq. (2) can be solved using different techniques, analytical and numerical method. So the dynamics of electrons in the SLs can be determined by solving the time-independent Schrödinger equation [10].

The solution of the Schrödinger Eq. (3) shows that there are an unlimited number of solutions for a given value of k , which is the Bloch wave number. Therefore, each wave function with a particular wavevector k is assigned a quantum number, n and has a corresponding energy $E^n(k)$; this function is known as the dispersion relation. The Bloch theorem then physically means that the wavefunction at position $x + X$ and x are the same, except for the phase factor $\exp(ikx)$. X is any translation vector of the lattice under consideration. Therefore, the Bloch's theorem tells us that the wave functions in one unit cell are related to those in the previous one simply by a phase factor of $\exp(ikx)$. Since, the wave function $u(x)$ must be periodic as Eq. (5),

$$u(x) = u(x + X) \quad (5)$$

the periodicity induced properties of the single-electron Schrödinger equation will then be

$$\left(-\frac{\hbar^2}{2m} \nabla^2 + V(x) \right) \psi(x) = E\psi(x) \quad (6)$$

if we substitute Eq. (2) into Eq. (6), the solution of Schrödinger equation will then be Eq. (7):

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V(x) \right] e^{ikx} u(x) = E e^{ikx} u(x) \quad (7)$$

and the function $u(x)$ satisfies the condition, for all

Fig. 1 Schematically structure of semiconductor superlattices. The superlattice unit cell consists of a quantum well (*GaAs*) enclosed by barriers (*AlAs*) [3].

vectors of lattice X , therefore the potential is periodic.

To obtain the dispersion relation energy $E^n(k)$ for the electron, we solve the Schrödinger equation for a single primitive cell of the SL. We use the Kronig-Penney model, which represents the one-dimensional periodic potential for the energy band. Fig. 2 shows an infinite periodic array of potential barriers with V_0 and an electron moving in the x -direction. Regions I and II represent well and barrier respectively. The potential function approximately equals to the square potential.

In the region, $0 < x < a$, the potential, $V = 0$ and the eigenfunction is as Eq. (8)

$$\psi = Ae^{iKx} + Be^{-iKx} \quad (8)$$

With the energy in the region described as

$$E = \frac{\hbar^2 K^2}{2m}$$

Similarly in the region, $-b < x < 0$, the solution will be as Eq. (9)

$$\psi = Ce^{Qx} + De^{-Qx} \quad (9)$$

We described the energy in the region as

$$V - E = \frac{\hbar^2 Q^2}{2m}$$

Using the Bloch theorem, the wavefunction would satisfy Eq. (10)

$$\psi(a < x < a + b) = \psi(-b < x < 0)e^{ik(a+b)} \quad (10)$$

and the boundary conditions at $x = 0$ and $x = a$ for

ψ and $\frac{d\psi}{dx}$ are to be continuous [11].

Let $\beta = \frac{Q}{K}$ and $d = a + b$

Therefore, we obtain:

$$\cos kd =$$

$$\cos Qb \cos ka + \frac{1}{2} \left(\beta - \frac{1}{\beta} \right) \sinh Qb \sin ka \quad (11)$$

This equation can be solved numerically for the dispersion relation in the miniband. Let represent the right hand of Eq. (11) as $f(\varepsilon)$ and expand it around the energy eigenvalue ε_j of an isolated well (that allows for narrow minibands), then Eq. (11) will become Eq. (12)

$$\cos kd = f(\varepsilon_j) + f'(\varepsilon_j)(\varepsilon - \varepsilon_j) \quad (12)$$

Fig. 2 The square well periodic potential, showing an electron moving in the x -direction against the Kronig-Penney potential (x). Region I is the well and region II is the barrier.

Solving for ε , gives Eq. (13)

$$\varepsilon = \varepsilon_j - f(\varepsilon_j)/f'(\varepsilon_j) + 1/f'(\varepsilon_j) \cos kd \quad (13)$$

The cosine dispersion is a good approximation for narrow minibands. The miniband dispersion is approximated by the cosine function with bandwidth, Δ and band edge ε_0 which can be derived from the dispersion relation in Eq. (11). Therefore, for the electron band, we write Eq. (14)

$$\varepsilon(k) \approx \varepsilon_0 - \frac{\Delta}{2}(1 - \cos(kd)) \quad (14)$$

3. Discussion and Conclusion

Esaki and Tsu in 1969 [1, 12] considered the idea of a one-dimensional SL, which is a periodic structure of layers of two or more materials. The materials have a similar lattice constant but a different band gap. The structure is formed by a periodic variation of alloy composition or impurity density introduced during epitaxial growth. These nanostructures consist of two or more different (typically two) semiconducting materials of similar lattice constants. The materials are deposited alternatively on each other to form a periodic structure in the growth direction [13, 14]. Nowadays the fabrication of these structures has been made possible by the development of epitaxial growth techniques such as MBE (molecular beam epitaxy). The process involves heating the pure element so that it sublimates. The resulting gaseous elements are

allowed to condense on a substrate to form a layer of the constituent atoms of that element. The process, crucially, is slow (around a monolayer per second) so that it is possible to precisely control the constituent atomic layers of the device, allow for the crystal to be tailored for specific experiments and applications [15, 16]. However, it is hard to grow materials with high vapour pressure using this process. Other types of epitaxial growth techniques are MOCVD (metal-organic chemical vapour deposition) and nanoscale lithography techniques (electron beam lithography) [17].

In the presence of external electric and magnetic fields the transport of electrons in minibands is a complex behavior which results in a number of interesting phenomena that have useful applications in the ultrafast electronics like THz Bloch oscillations [1, 18], dynamical electron confinement, negative differential velocity [19], and cyclotron-Bloch resonances and dynamical chaos [20]. These properties of SLs derive from a number of periodic layers that can be structured and controlled as desired. The chemical composition of SLs varies periodically in space at distances of (1-10 nm) which is greater than the periods of its constituent materials. This man-made structure is made to investigate a fundamental quantum mechanical phenomenon that forms quantised energy states [21-23]. Since the thickness of the layers, the number of periods and periodic potential strength can be controlled [16]. The motion of electrons in the SLs is modified by the arrangement of the atoms in a periodic way. The magnitude of the band gap of the SLs can be tuned and the parameters of the materials can be varied, which optimizes and widens its applications.

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