Appearance of Pseudo-Band-Gaps in a Disordered Quantum Wire Array

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Abstract

The density of states and the conductivity are calculated in lateral superlattices with disorder in the period within a self-consistent Born approximation. Although the potential loses its periodicity on average due to disorder, it leads to an opening up of a pseudo-band-gap and modifies the conductivity perpendicular to the superlattice even qualitatively, when the energy reaches the zone boundary.

Key words: Lateral superlattice, Anisotropic mobility, Periodic corrugation, Bragg scattering

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1. Introduction

A periodic quantum-wire array was formed during growth of a GaAs/AlAs heterointerface on a GaAs (775)B substrate by molecular beam epitaxy [1–3]. This was achieved by the growth of corrugated GaAs quantum well with a zigzag shape on top of a flat AlAs surface and covered by an AlAs barrier layer. Figure 1 gives a schematic illustration of the structure. The purpose of this paper is to explore the transport of such strongly modulated two-dimensional systems theoretically.

In transport experiments a large anisotropy was observed, in which the conductivity in the direction parallel to the wires is more than one order of magnitude larger than that in the perpendicular direction [3,4]. The opening-up of a band gap due to a periodic potential was suggested as the origin of the observed large anisotropy [3]. However, a self-consistent calculation of electronic states showed that the gap is not so large and the Fermi level lies lower than the zone boundary [5]. As a result, the energy dispersion is almost circularly symmetric and band-structure effects like anisotropic effective masses cannot explain the experiments [5]. Actual zigzag corrugations have some fluctuations. Effects of disorder in the period and height of the periodic potential were calculated to the lowest order using a Boltzmann equation and could successfully explain the large anisotropy [6,7].

When the energy approaches the zone boundary, an electron suffers from strong diffuse Bragg scattering and the lowest order approximation based on the Boltzmann equation is likely to become invalid. In fact, an electron can feel the presence of a coherent potential for several periods when the disorder is not extremely large, leading to the formation of a pseudo-
band-gap. In this paper we calculate the density of states and transport coefficients of this disordered one-dimensional superlattice including effects of fluctuating corrugation in a self-consistent Born approximation and study effects of such pseudo-gap formation on the transport.

2. Disorder in Periodic Corrugation

Let $\Delta(r)$ be a periodic interface corrugation. When it has a perfect periodicity in the $x$ direction, we can expand $\Delta(r)$ as

$$\Delta(r) = \sum_n \Delta_n \exp\left(\frac{2\pi i n x}{a}\right),$$  \hspace{1cm} (1)

where $a$ is the period. For the corrugation of a triangular shape we have

$$\Delta_n = \Delta \left(\frac{1}{2\pi n}\right)^2 \frac{a^2}{a_1 a_2} \left[1 - \exp\left(-i \frac{2\pi n a_1}{a}\right)\right],$$  \hspace{1cm} (2)

for $n \neq 0$ and $\Delta_n = 0$ for $n = 0$, where $a_1/a = 1/3$ and $a_2/a = 2/3$. Qualitative results are essentially the same for other corrugations.

We consider the situation that the period exhibits a fluctuation whose amount $\alpha$ is much smaller than the period itself, i.e., $\alpha/a \ll 1$. We assume that there is approximately no correlation between fluctuations of different periods. We assume further that the local tilt angle of the corrugation exhibits a Gaussian distribution with width $\nabla \xi \equiv \sqrt{\langle (\partial \xi/\partial y)^2 \rangle}$ and that the average height $\Delta_0$ varies along the quantum-wire direction slowly with correlation length $\lambda$ and average fluctuation $\Delta_0$.

Then, the average corrugation vanishes identically, i.e., $\langle \Delta(r) \rangle = 0$. The correlation function is given by [6]

$$D(r-r') \equiv \langle \Delta(r)\Delta(r') \rangle$$

$$= \Delta^2 \int \frac{d\mathbf{q}}{2\pi} g(q) \exp[iq(x-x')]$$

$$\times \exp\left[-\frac{1}{2} \left(\nabla \xi^2 q^2 + \frac{2}{\lambda^2} (y-y')^2\right)\right] + \sum_{n \neq 0} |\Delta_n|^2 \exp\left[i \frac{2\pi n (x-x')}{a}\right]$$

$$\times \exp\left[-\frac{1}{2} \left(\frac{2\pi n}{a}\right)^2 \left(\alpha^2 \frac{|x-x'|}{a} + \nabla \xi^2 (y-y')^2\right)\right],$$  \hspace{1cm} (3)

with $g(q) = [4a/(qa^2)]^2 \sin^2(qa/2)$. The most important feature is the exponential decay in the $x$ direction and that the decay rate is determined by the amount of fluctuations in the period.

The effective potential due to the corrugation takes the form as $V(r) = F_{\text{eff}} \Delta(r)$. In quantum-well cases we have $F_{\text{eff}} = \partial E_0(\bar{d})/\partial \bar{d}$, where $E_0(\bar{d})$ is the energy of the lowest subband in the quantum well with average width $\bar{d}$ [8,9]. In a single heterostructure, $F_{\text{eff}}$ is the effective field at the interface [10–12].

The tilt angles $\theta_1$ and $\theta_2$ of a corrugation are likely to be determined by the microfacets appearing during the growth process, while the height of the peak and valley of the corrugation is likely to vary almost at

![Fig. 1. A schematic illustration of a periodic quantum-wire array consisting of a GaAs/AlAs heterostructure. The quantum wires are along the $y$ direction.](image)

![Fig. 2. An example of the correlation function $D(q)$.](image)
random between neighboring corrugations. For such a random fluctuation of the bottom and peak heights \( \Delta z = \sqrt{\langle z^2 \rangle} \), we have

\[
\Delta_0^2 = \frac{\Delta z^2}{4a^2} (a_1^2 + a_1 a_2 + a_2^2), \quad \alpha^2 = \frac{2 \Delta z^2}{\Delta z} (a_1^2 + a_1 a_2 + a_2^2) .
\]  \( \quad (4) \)

Figure 2 shows an example of the Fourier transform \( D(q) \) of \( D(r) \) for \( \Delta z/\Delta = 0.1 \) [eq. (2.33) of ref. [6] seems to contain an error]. An important feature is the presence of a large Bragg peak at \( q = (\pm 2\pi/a, 0) \) broadened in the \( q_x \) direction by a Lorentzian function corresponding to the exponential decay in the real space. In the \( q_y \) direction the correlation function is essentially given by a Gaussian, but its actual form varies as a function of \( q_x \).

3. Self-Consistent Born Approximation

In a self-consistent Born approximation, the self-energy \( \Sigma(k, E) \) of the averaged Green’s function \( G(k, E) \) is given by

\[
\Sigma(k, E) = \int \frac{dq}{(2\pi)^2} [F_{0k}^2 D(q) + n_iu_i^2]G(k - q, E). \]  \( \quad (5) \)

In the above, we have introduced short-range scatterers \( \sum_i u_i \delta(r - r_i) \) with concentration \( n_i \) in a unit area, where \( r_i \) denotes the position of the \( i \)th scatterer. The conductivity can be calculated by solving a Bethe-Salpeter-type equation for vertex corrections [13], consistent with the approximation for the self-energy.

Because of the explicit and strong dependence of the self-energy on the wave vector, a self-consistency is achieved only through discretization of the wave-vector space. Short-range scatterers have to be introduced because of the practical reason that a solution of the above equation should accurately be obtained. Their strength is characterized by the mean free path \( \Lambda_0 = v_0\tau_0 \) with the velocity at the zone boundary \( v_0 = \pi \hbar/m^*a \) and the relaxation time \( \tau_0 \) given by \( \hbar/2\tau_0 = n_iu_i^2m^*/2\pi\hbar^2 \), where \( m^* \) is the effective mass.

4. Results

Figure 3 shows some examples of calculated density of states in the vicinity of \( \varepsilon_0 = (\hbar^2/2m^*)/(\pi/a)^2 \) corresponding to the first zone boundary. The density of states is normalized by that of two-dimensional free electrons, \( D_0 = m^*/\pi\hbar^2 \). For a small disorder in the corrugation \( \alpha/a = 0.06 \), the density of states exhibits a characteristic feature corresponding well to the formation of a gap, although broadened considerably due to the disorder and the presence of short-range scatterers. This feature is smoothed out with the increase of the disorder and disappears completely for \( \alpha/a > 0.25 \).

Figure 4 shows corresponding results for the conductivity in the \( x \) (\( \sigma_{xx} \), perpendicular to quantum wires) and \( y \) direction (\( \sigma_{yy} \), parallel to quantum wires) as a function of the Fermi energy. The conductivity is normalized by the Boltzmann result \( \sigma_0 = n_ee^2\tau_0/m^* \) determined by short-range scatterers, where the electron concentration is given by \( n_0 = \varepsilon_0D_0 \).

The anisotropy of the conductivity when the Fermi energy is about a half of \( \varepsilon_0 \) (roughly corresponding to the actual experimental conditions [3,4]) is much smaller than that obtained previously [6,7]. This is a direct consequence of the presence of strong short-
Fig. 4. Examples of calculated conductivity as a function of the Fermi energy for various values of the disorder in corrugation in the presence of short-range scatterers characterized by $\Lambda_0/a=16$.

range scatterers giving isotropic transport. When the energy approaches the zone boundary, the conductivity $\sigma_{xx}$ has a prominent dip due to the strong diffuse Bragg scattering. The amount of the dip is about the same (actually slightly smaller) as that calculated using the Boltzmann equation in the presence of short-range scatterers.

The most notable feature is that $\sigma_{yy}$ has a broad and weak peak in the vicinity of the zone boundary quite in contrast to a considerable dip obtained previously in the Boltzmann transport theory [6,7]. This appearance of the peak in $\sigma_{yy}$ arises due to the formation of a pseudo-gap due to the strong diffuse Bragg scattering. However, a part of the reason for the disappearance of the dip lies again in the presence of strong short-range scatterers. In fact, the Boltzmann $\sigma_{yy}$ has only a broad and tiny dip-structure, showing that $\sigma_{yy}$ is still governed by short-range scatterers.

It turns out, under the present circumstances, that the Boltzmann conductivity is valid except for the small difference (qualitatively important for the conductivity parallel to wires but quantitatively not so significant) in the vicinity of the zone boundary. An important issue left for the future is whether the conductivity parallel to wires has a dip or peak when the strength of short-range scatterers is sufficiently small and the transport is dominated by the diffuse Bragg scattering.

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References