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1995 J. Phys.: Condens. Matter 7 9811

(http://iopscience.iop.org/0953-8984/7/50/015)

J. Phys.: Condens. Matter 7 (1995) 9811–9817. Printed in the UK

Convective instability of a biased semiconductor superlattice

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Received 12 May 1995, in final form 6 September 1995

Abstract. A fully three-dimensional analysis of the convective instability of a planar superlattice biased in the regime of negative differential miniband conductance is carried out for the first time with accurate microscopic treatment of phonon and impurity scatterings. For a typical GaAs-based superlattice having period $d = 10$ nm, miniband width $\Delta = 900$ K and electron sheet density $N_s = 1.5 \times 10^{15}$ m^{-2}, we find that the convective space-charge waves propagate at a phase velocity ranging from $0.75v_0$ to $0.95v_0$ (v_0 is the carrier drift velocity) and with an amplitude growth rate only about a few per cent of that predicted by the conventional drift-diffusion model and other existing methods.

Negative differential mobility (NDM) in vertical superlattice transport, predicted a quarter of a century ago by Esaki and Tsu [1] and recently observed [2–4], has attracted much attention in the literature [5–8]. NDM has not only brought into focus the prospect of realizing a superlattice microwave oscillator, spurring on studies of miniband response at high frequency [9–12], but it is also intimately related to instability of the uniform distribution of electric field in superlattices. Unlike narrow-miniband systems in which the salient transport inhomogeneity shows up in the formation of high-field domains and in periodic structure of the I–V characteristic when the applied voltage surpasses a threshold [13–16], the most interesting conduction phenomena in wide-miniband superlattices are those related to Esaki–Tsu NDM at relatively low electric field. The basic physical features of these Bragg-diffraction-related phenomena follow from a one-dimensional band structure. Nevertheless, carrier scatterings by impurities, by phonons and among themselves make the problem truly three dimensional (3D). The existing nonuniform models [17, 18], using constant relaxation times in place of the scattering contributions and being essentially one dimensional (1D) in nature, are not sufficient for a quantitative examination of miniband conduction. In this paper we report a fully three-dimensional analysis of miniband transport for a planar superlattice, treating both spatial inhomogeneity and realistic scattering mechanisms, within the framework of a 3D balance-equation approach [6, 19–22].

Consider an infinite GaAs-based planar superlattice in which electrons move freely in the transverse (x–y) plane and can travel along the growth axis (z-direction) through the (lowest) miniband formed by periodic potential wells and barriers of finite height. The electron energy dispersion can be written as the sum of a transverse energy $\varepsilon_{k_\parallel} = k_\parallel^2/2m$ (m

being the band mass of the carrier in the bulk semiconductor), and a tight-binding miniband energy $\varepsilon(k_z)$ related to the longitudinal motion:

$$\varepsilon(\boldsymbol{k}) = \varepsilon_{\boldsymbol{k}_\parallel} + \varepsilon(k_z) \tag{1}$$

with

$$\varepsilon(k_z) = (\Delta/2)(1 - \cos k_z d) \tag{2}$$

where $\boldsymbol{k} = (\boldsymbol{k}_\parallel, k_z)$, $\boldsymbol{k}_\parallel = (k_x, k_y)$ represents the in-plane wavevector: $-\infty < k_x, k_y < \infty$, and $-\pi/d < k_z \leqslant \pi/d$, d being the superlattice period along the z-direction, and Δ is the miniband width.

In the balance-equation transport theory for an arbitrary energy band [19, 20], the transport state of a many-electron system is described by the average (per carrier) centre-of-mass momentum p_d and the electron temperature T_e. In spatially homogeneous cases, the acceleration and the energy-balance equations completely determine the system response to either constant or time-dependent uniform electric fields. For the spatially inhomogeneous case, in addition to p_d and T_e, we employ also ζ (the ratio of the chemical potential to T_e) as a fundamental variable, and treat p_d, T_e and ζ, and correspondingly the carrier number density n, the average drift velocity v_d and all other quantities, as being time and space dependent [21, 22]. Considering balances of the carrier number density, the acceleration and the energy in a small volume element around a spatial position, we obtain hydrodynamic balance equations of the following type for superlattice vertical transport, in which the electric field and the carrier drift are assumed in the z-direction, $\boldsymbol{E} = (0, 0, E)$, $\boldsymbol{p}_d = (0, 0, p_d)$ and $\boldsymbol{v}_d = (0, 0, v_d)$, with spatial inhomogeneity only along the superlattice z-axis:

$$\frac{\partial n}{\partial t} = -\frac{\partial}{\partial z}(n v_d) \tag{3}$$

$$\frac{\partial}{\partial t}(n v_d) = -\frac{\partial}{\partial z}(n B_z) + \frac{n e E}{m_z^*} + n A \tag{4}$$

$$\frac{\partial}{\partial t}(n \epsilon) = -\frac{\partial}{\partial z}(n S_z) + n e E v_d - n W. \tag{5}$$

Here, n is the average carrier density, ϵ the average carrier energy, v_d the average carrier drift velocity, $1/m_z^*$ the zz-component of the inverse effective-mass tensor, B_z the zz-component of the average velocity–velocity dyadic, and S_z the z-component of the energy flux vector. They are functions of $z_d \equiv p_d d$, T_e, and ζ, and thus are time and space dependent through these fundamental variables. In these equations the frictional acceleration $A = A_i + A_p$ (due to impurity and phonon scatterings), and the energy-loss rate (per particle) W (due to phonon scattering) are given by the same expressions as those given in [6]. For a superlattice system with known impurity distributions and phonon modes and known electron–impurity potentials and electron–phonon coupling matrix elements, A and W, are completely determined by z_d, T_e and ζ.

The electric field relates to space charge through its divergence in accordance with the Gauss theorem (Poisson equation):

$$\frac{\partial E}{\partial z} = \frac{e}{\epsilon_0 \kappa}(n - n_0) \tag{6}$$

where e is the electron charge, κ is the dielectric constant of the semiconductor, and n_0 is the background density of positive charge which is assumed to be uniformly distributed over the whole superlattice. This equation shows that if the electric field is uniformly distributed, $\partial E/\partial z = 0$, the electron charge density is $n = n_0$.

With the miniband energy dispersion of equation (1), n, v_d, $1/m_z^*$, B_z and S_z can be written explicitly as follows:

$$n = n_0\alpha_0(T_e, \zeta) \tag{7}$$

$$nv_d = n_0 v_m \alpha_1(T_e, \zeta)\sin z_d \tag{8}$$

$$n/m_z^* = (n_0/M^*)\alpha_1(T_e, \zeta)\cos z_d \tag{9}$$

$$nB_z = n_0(v_m^2/2)[\alpha_0(T_e, \zeta) - \alpha_2(T_e, \zeta)\cos 2z_d] \tag{10}$$

$$nS_z = n_0(v_m\Delta/2)[\alpha_1(T_e, \zeta)\sin z_d - \tfrac{1}{2}\alpha_2(T_e, \zeta)\sin 2z_d + \beta_1(T_e, \zeta)\sin z_d] \tag{11}$$

and

$$n\epsilon_z = n_0(\Delta/2)[\alpha_0(T_e, \zeta) - \alpha_1(T_e, \zeta)\cos z_d] \tag{12}$$

$$n\epsilon_\parallel = n_0(\Delta/2)\beta_0(T_e, \zeta) \tag{13}$$

with $\epsilon = \epsilon_z + \epsilon_\parallel$. In the above, $v_m \equiv \Delta d/2$, $1/M^* = \Delta d^2/2$, $\alpha_0(T_e, \zeta) = \langle 1\rangle_0$, $\alpha_1(T_e, \zeta) = \langle\cos(k_z d)\rangle_0$, $\alpha_2(T_e, \zeta) = \langle\cos(2k_z d)\rangle_0$, $\beta_0(T_e, \zeta) = \langle(k_\parallel^2/m\Delta)\rangle_0$, $\beta_1(T_e, \zeta) = \langle(k_\parallel^2/m\Delta)\cos(k_z d)\rangle_0$, and $\langle\ldots\rangle_0$ stands for the average

$$\langle\ldots\rangle_0 = \frac{1}{4\pi^3 n}\int\int \mathrm{d}k_x\,\mathrm{d}k_y \int_{-\pi/d}^{\pi/d} \mathrm{d}k_z\ f(\varepsilon(k)/T_e - \zeta)\ldots$$

with $f(x) = 1/[\exp(x) + 1]$ being the Fermi distribution function.

To investigate the dynamic mobility and proceed with the mode analysis under drifted conditions we consider small wavelike fluctuations: δz_d, δT_e, $\delta\zeta$, δv_d and $\delta Q \sim \exp[\mathrm{i}(kz - \omega t)]$ (Q stands for E, n, $1/m_z^*$, B_z, S_z, ϵ, ϵ_z, or $\epsilon_\parallel$), superimposed on the corresponding dc bias quantities such that $z_d = z_0 + \delta z_d$, $T_e = T_0 + \delta T_e$, $\zeta = \zeta_0 + \delta\zeta$, $v_d = v_0 + \delta v_d$, and $Q = Q_0 + \delta Q$.

In the zeroth order, the continuity equation (3) and the Poisson equation (6) are identities, and the other two equations are just the dc steady-state equations for the effective force and energy balance in the spatially homogeneous case:

$$0 = eE_0/m_{z0}^* + A_0 \tag{14}$$

$$0 = eE_0 v_0 - W_0 \tag{15}$$

where

$$v_0 = v_m\alpha_{10}\sin z_0 \tag{16}$$

$$1/m_{z0}^* = (1 - 2\epsilon_{z0}/\Delta)/M^* \tag{17}$$

$$\epsilon_{z0} = (\Delta/2)(1 - \alpha_{10}\cos z_0) \tag{18}$$

and

$$1 = \alpha_0(T_0, \zeta_0). \tag{19}$$

Here we have used the notation $\alpha_{10} \equiv \alpha_1(T_0, \zeta_0)$, $A_0 \equiv A(z_0, T_0, \zeta_0)$, and $W_0 \equiv W(z_0, T_0, \zeta_0)$. Equation (19) determines ζ_0 as a function of T_0 in the spatially homogeneous condition. The solutions of the equations (14) and (15) have been discussed in [6]. The dependence of the bias drift velocity v_0 as a function of the bias electric field E_0 on the miniband width, superlattice period, carrier density, lattice temperature and strength of impurity scattering have been examined in some detail for n-type GaAs systems [6].

As an example, we consider a GaAs-based superlattice with period $d = 10$ nm, miniband width $\Delta = 900$ K, carrier sheet density $N_s = 1.5 \times 10^{15}$ m^{-2}, and low-temperature linear dc mobility $\mu(0) = 1.0$ m^2 V^{-1}s^{-1} at lattice temperature $T = 300$ K. The dc steady-state drift

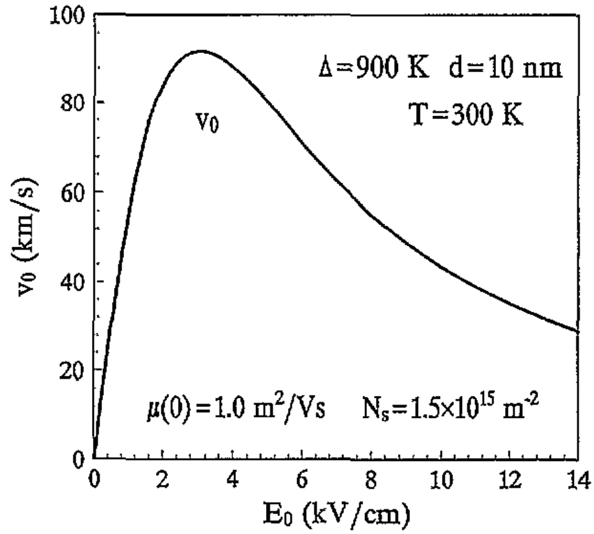

Figure 1. The drift velocity v_0 in dc steady-state transport, as determined by equations (14) and (15), is shown as a function of the applied field E_0 at lattice temperature $T = 300$ K, for a GaAs-based superlattice with period $d = 10$ nm, miniband width $\Delta = 900$ K, carrier sheet density $N_s = 1.5 \times 10^{15}$ m^{-2} and low-temperature linear dc mobility $\mu(0) = 1.0$ m^2 V^{-1} s^{-1}.

velocity as a function of electric field (v_0 versus E_0) obtained from the zero-order balance equations (14) and (15) is shown in figure 1.

The balance equations for linear order fluctuations can be written in terms of four variables: δz_d, δT_e, $\delta\zeta$ and δE, and they form a set of four homogeneous linear algebraic equations. The coefficients of this set of equations are obtained in a straightforward manner, but the expressions for them are rather lengthy. We omit them here in the interests of brevity. For this set of linear algebraic equations to have a nonzero solution requires that their determinant vanishes:

$$\mathcal{D}(k, \omega) = 0. \tag{20}$$

This determines the dispersion relation between k and ω for all the eigenmodes of the system.

In the spatially uniform case, $k = 0$, equation (20) yields $\mathcal{D}(0, \omega) = 0$, which is satisfied for arbitrary ω. Therefore, we can, in principle, apply a small uniform ac field δE of (real) frequency ω superimposed on a bias dc field E_0, and consider the velocity response δv_d of the system. The small-signal (complex) mobility is defined as

$$\mu_\omega = \frac{\delta v_d}{\delta E}. \tag{21}$$

The real part of this small-signal mobility in the space-uniform case, $\mathrm{Re}\,\mu_\omega$, calculated for the system described above, is shown in figure 2 as a function of frequency $\nu \equiv \omega/2\pi$ of the ac driving field at several different dc biases E_0 ranging from 0.2 to 15 kV cm^{-1}.

In the spatially inhomogeneous case of $k \neq 0$, equation (20) can be satisfied generally only for complex $k = k_1 + ik_2$ and/or complex $\omega = \omega_1 + i\omega_2$. We concentrate here on the most interesting drift-relaxational modes and related instabilities and examine the case of a real wavevector: $k = k_1$ and $k_2 = 0$. The real wavevector k_1 and the imaginary part of the frequency, ω_2, obtained from equation (20) as functions of the real frequency $\nu = \omega_1/2\pi$ are shown, respectively, in figures 3 and 4 for several dc bias fields E_0 from 2.0 kV cm^{-1}

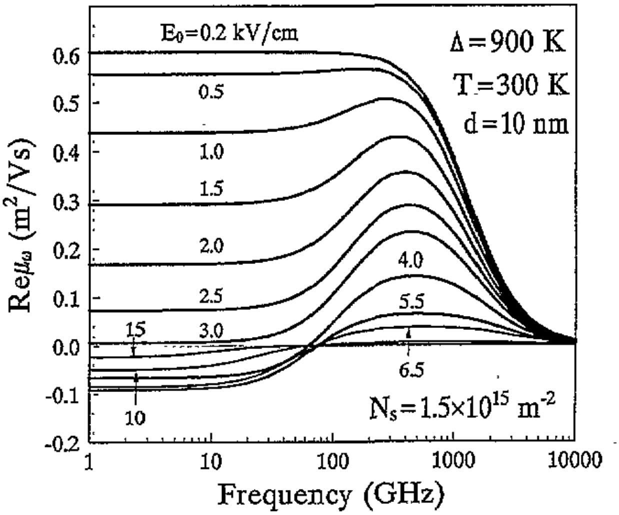

Figure 2. The real part of the small-signal mobility in the spatially uniform case, $\mathrm{Re}\,\mu_\omega$, is shown as a function of the signal frequency $\nu = \omega/2\pi$ for the GaAs-based superlattice as described in figure 1, at lattice temperature $T = 300$ K with the bias electric field E_0 ranging from 0.2 to 15 kV cm^{-1}.

to 7.0 kV cm^{-1}. When biased in the NDM regime, ω_2 is positive for low ω_1 (low k), and continues to be positive with increasing frequency until ω_1 reaches a maximum value dependent on the bias. A positive ω_2 implies a travelling wave

$$\exp[\omega_2 t + \mathrm{i}(k_1 z - \omega_1 t)] \tag{22}$$

propagating along the positive z-direction with its amplitude growing exponentially as a function of time. The phase velocity of this space-charge wave, $v_{ph} = \omega_1/k_1$, can be obtained from figure 3 and is shown in the inset of this figure. Depending on the bias and frequency, v_{ph} varies from $0.75v_0$ to $0.95v_0$, v_0 being the bias drift velocity.

The convective instability in semiconductors exhibiting NDM has usually been analysed using a phenomenological drift-diffusion (DD) model [23], which yields a dispersion relation for real $k = k_1$ ($k_2 = 0$) of the form

$$\omega = v_0 k - \mathrm{i}(\omega_c + Dk^2) \tag{23}$$

where

$$\omega_c = (en_0/\epsilon_0\kappa)\mu_0 \tag{24}$$

with $\mu_0 = \partial v_0/\partial E_0$ being the zero-frequency differential mobility and D a diffusion constant. Equation (23) describes a convective space-charge wave having a phase velocity equal to the carrier drift velocity v_0 and an imaginary frequency component $\omega_2 = -\omega_c$ at small wavevector. Earlier balance-equation methods yield essentially the same behaviour for small k [17, 18]. The present 3D analysis, however, leads to a significantly different result: convective space-charge waves propagate at a phase velocity varying from $0.75v_0$ to $0.95v_0$ and with an imaginary frequency ω_2 of about 1.9 to 3.8% (for E_0 from 4.0 to 7.0 kV cm^{-1}) of $|\omega_c|$ (equation (24)) calculated from zero-frequency mobility μ_0.

One should not be overly surprised by these results. The hydrodynamic balance equations we have employed to analyse the space-charge-wave modes are considerably more sophisticated than the drift-diffusion (DD) model previously used in the literature. The

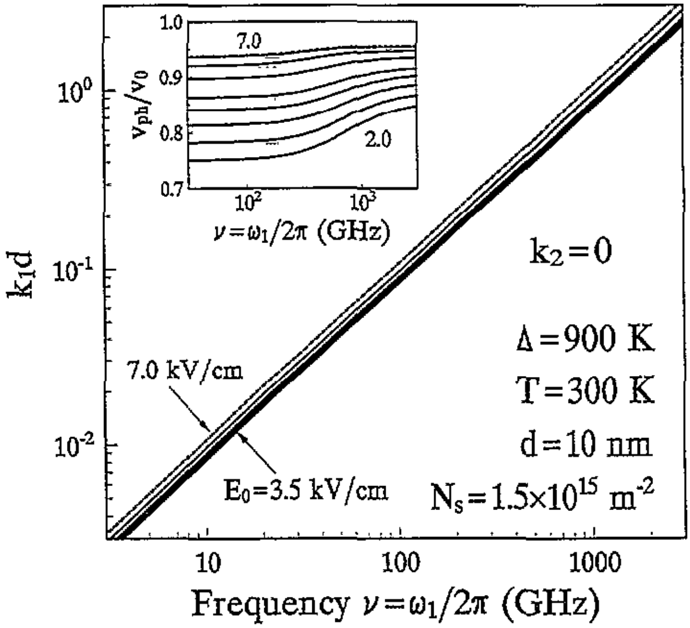

Figure 3. The real wavevector parameter, k_1d, obtained from dispersion equation (20) in the case where $k_2 = 0$ is plotted as a function of real frequency $\nu = \omega_1/2\pi$ at lattice temperature $T = 300$ K under several different dc bias fields, for the same GaAs-based superlattice as described in figure 1. The inset shows the phase velocity v_{ph} in units of bias drift velocity v_0 as a function of ν under different dc bias fields ranging from 2.0 to 7.0 kV cm^{-1}.

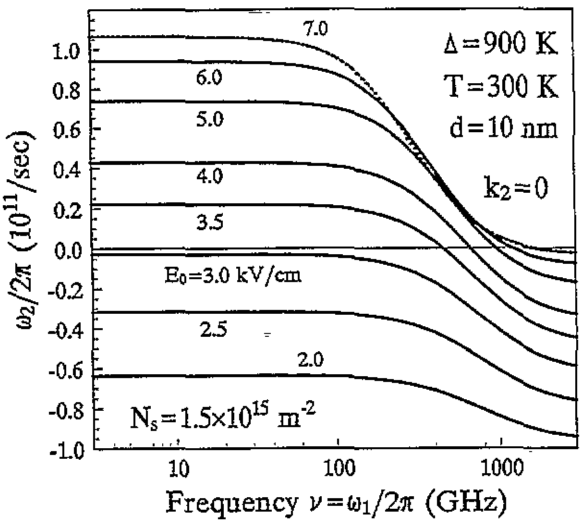

Figure 4. The imaginary frequency parameter, $\omega_2/2\pi$, obtained from dispersion equation (20) in the case where $k_2 = 0$ is shown as a function of real frequency $\nu = \omega_1/2\pi$ for the same GaAs-based superlattice as described in figure 1 at lattice temperature $T = 300$ K under several different dc bias fields.

phenomenological DD model is based on the assumption that the system exhibits NDM and has a very short momentum relaxation time. It takes partial account of the effects of spatial inhomogeneity only through the carrier-density-associated diffusion term, but disregards spatial variations of the electron temperature and centre-of-mass variables. The DD model is also deficient in that it completely ignores energy balance—hence the frequency dependence of the ac mobility in the spatially uniform case is neglected, while this is vital in high-field miniband transport. The present hydrodynamic-balance-equation approach, which takes proper account of the energy balance and provides a unified description of dc steady-state, high-frequency and spatially inhomogeneous transport, is quite different from the DD model. In this balance-equation approach there is an energy relaxation time which is an order of magnitude larger than the momentum relaxation time, so the ac mobility exhibits a strong frequency variation at relatively low frequency. Furthermore, spatial inhomogeneity is considered through all the variables involved. These are the physical reasons for the present balance-equation predictions for the convective space-charge wave differing from those of the DD model. Nevertheless, the present hydrodynamic model still predicts the existence of unstable convective space-charge waves, in qualitative agreement with the DD model. This suggests that Gunn-like phenomenology due to Bragg-scattering-induced NDM may occur in wide-miniband superlattices. Previously explored one-dimensional models, which yield essentially the same results as the DD model, are not sufficient for a quantitative analysis. The full 3D hydrodynamic balance equations (3)–(5) introduced here provide convenient and more accurate tools for dealing with these miniband effects.

Acknowledgments

The authors are grateful to Dr K K Thornber for valuable discussions. They also thank the National Natural Science Foundation of China, National and Shanghai Municipal Commissions of Science and Technology of China, and the Army Research Office of the United States for support of this work.

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