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Energy Spectrum of Thin Film Heterostructure

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Using the Green's function method the charge carrier energy spectrum in a thin film heterostructure is studied taking account of the surface states. The density of states in various parts of the heterostructure is calculated. It is shown that their ratio may vary within large limits. This may lead to the appearance of a negative conductivity in presence of a longitudinal electric field.

На основе метода функции Грина исследуется энергетический спектр носителей заряда в тонкопленочной гетероструктуре с учетом поверхностных состояний. Вычисляется плотность состояний в различных частях гетероструктуры. Показано, что их отношение может меняться в довольно широких пределах. Это может привести к возникновению отрицательной дифференциальной проводимости в присутствии продольного электрического поля.

1. Introduction

Investigation of thin heterostructure (TFH) attracts increasing attention at present. The study of the energy spectrum of the charge carriers with account taken of the film or surface states is of great interest, since the states may notably influence the electric, photoelectric, and other properties of the system (see, for example [1, 2]). Thus the density of states and the mobility may vary considerably from one part of the TFH to the other. Hence the negative conductivity may be obtained in TFH [3] in high enough electric fields, somewhat analogous to the Gunn effect. In connection with this it is interesting to study the density of states in various parts of the TFH taking account of the quantum size effect.

2. Results and Discussion

Generally the TFH may be viewed as a four-subsystem structure (see Fig. 1). The microscopic characteristics of the exterior subsystems depend essentially upon the boundary conditions at the interfaces. We treat the inner subsystems as thin ideal crystals called further film 1 and film 2 of width d_1 and d_2 , respectively; there is generally a transition region between them. For simplicity we assume the heterojunction to be sharp and neglect the width of the transition region. This assumption is correct if the width of the transition region is small enough compared to d_1 and d_2 (in the energy region corresponding to the bands of separate crystals) and to the localization radii of the interface states (within the gap).

Let the TFH have two-dimensional translation invariance and let the boundary surfaces of the TFH represent the symmetry planes of each crystal. Then for small values of a two-dimensional wave vector k_{\perp} directed along the boundary planes the three-dimensional problem may be reduced in a good approximation to the one-dimensional

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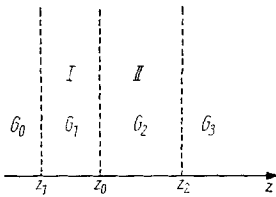


Fig. 1. The scheme of the one-dimensional four-subsystem structure

one [4, 5]. Therefore we shall consider the problem in the one-dimensional form. Transition to the three-dimensional case may be made by replacing the one-dimensional Green's function (GF) by a surface GF, which depends upon the parameters \mathbf{k}_\perp .

We assume that the GF's ($G_j(z, z'; E)$, $j = 0, 1, 2, 3$) for both subsystems are known. The density of states and the energy levels for such a structure are determined by the GF of the four interacting subsystems (i.e. by a three-junction GF). The poles of the latter are given by the roots of the equation ($\hbar = 2m_0 = 1$)

$$D(E) = 1 - \lambda_1 r_{10} r_{12} - \lambda_2 r_{21} r_{23} - \lambda_1 \lambda_2 r_{10} r_{23} (1 - r_{21} - r_{12}) = 0. \quad (1)$$

Here the complex reflection amplitudes r_{ij} are expressed in terms of the function G_j [6]:

$$\lambda_j = [G_j(z_j, z_0) G_j(z_0, z_j)] [G_j(z_j, z_j) G_j(z_0, z_0)]^{-1}.$$

The amplitudes r_{10} and r_{23} act as the boundary condition, while r_{12} and r_{21} describe the interaction between the interior subsystems forming the heterostructure.

Interface or contact states arising at the boundary of the two systems in a common gap are determined by the poles of the amplitudes r_{10} , r_{23} , and r_{12} (or r_{21}). The positions of these levels depend essentially upon the matching conditions [7, 8], therefore, in a real crystal the states should be distributed over the gap [9]. If the width of each film of the TFH is assumed to be sufficiently larger than the localization radius of the states, then the latter may be considered as independent, i.e. they may be obtained from the solution of the one-junction problem. The position of the film levels within the bands of both films depends but weakly on the boundary conditions [10]. Therefore, one may assume for simplicity that the exterior subsystems are impenetrable for the carriers, i.e. complete reflection takes place: $r_{10} = r_{23} = 1$. Then (1) takes the form

$$\frac{G'_1 + i \operatorname{ctg} k_1 d_1}{G_1} = \frac{G'_2 - i \operatorname{ctg} k_2 d_2}{G_2}, \quad (2)$$

where

$$2k_1 d_1 = \int_{z_1}^{z_0} \frac{i dz}{G_1(z, z)}, \quad 2k_2 d_2 = \int_{z_0}^{z_2} \frac{i dz}{G_2(z, z)},$$

$$d_1 = z_0 - z_1 = m a_1, \quad d_2 = z_2 - z_0 = n a_2, \quad (2a)$$

z_1 and z_2 are the boundary planes of the TFH, z_0 is the contact plane of the heterostructure; a_1 and a_2 are lattice constants of the films; m and n are integers; $G_j = G_j(z_0, z_0)$, $G'_j = (\partial/\partial z_0) G_j(z_0, z_0)$.

Equation (2) is written for the case when the energy takes on values from the common gap of the two subsystems. The quantities k_j ($j = 1, 2$) are the electron wave numbers in the corresponding subsystems, given by (2a). In the energy region which is forbidden in one of the films (say, the first) the energy spectrum is obtained from (2) where k_1 is to be replaced by $i\kappa_1$ ($\kappa_1 > 0$). Another analytical continuation $k_2 = i\kappa_2$ ($\kappa_2 > 0$) is needed to consider the states in the common gap of both subsystems.

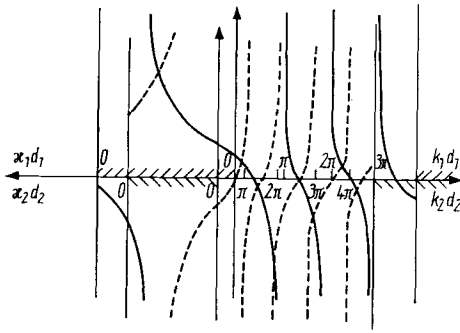


Fig. 2. Qualitative curves of the left-hand side (full curves) and the right-hand side (broken curves) of equation (2). The values $k_j = \alpha_j = 0$ correspond to the band edges (E_{vj} , E_{cj}) of the j -th film. The regions corresponding to the gaps are hatched

Thus the problem of calculating the energy of the surface and film states is reduced to obtaining the graphical solutions of equation (2). For an arbitrary periodic potential it is possible to obtain the qualitative curves of both parts of (2), which depend upon the values of energy and the parameter z_0 . To draw the graph of the left-hand side it is necessary to know the positions of E_0 in the gap ($G_1(z_0, z_0; E_0) = 0$) and of the asymptotes in the band $k_1 d_1 = n\pi$, $n = 1, 2, 3, \dots$ (see Fig. 2, full line). The intersection of these curves with the corresponding right-hand side curves (the broken line) gives the energy levels required. The parameters of both subsystems being known the energy levels may be obtained in the whole region of interest. For the sake of simplicity we consider the case when the periodic potentials of the crystals reach their extrema at the three boundaries of the TFH. Then $G'_j = 0$ and we obtain a compact formula for the density of states in various films

$$\rho_I(E) = \frac{1}{d_1} \frac{D'_1}{D'} \sum_n \delta(E - E_n), \quad \rho_{II}(E) = \frac{1}{d_2} \frac{D'_2}{D'} \sum_n \delta(E - E_n). \quad (3)$$

Here D'_j is the derivative of

$$D(E) = G_1 \operatorname{tg} k_1 d_1 + G_2 \operatorname{tg} k_2 d_2, \quad (4)$$

with respect to the energy for the j -th film, E_n are the energy levels determined by the condition $D(E_n) = 0$. Note that in the different TFH films the coefficients of the δ -functions, and thus the expressions for the density of states, are different. Their ratio at $E = E_n$ may vary within a broad range. Once the conditions are satisfied for the first subband to be filled and $A_1 \gg 1$, $\mu_2 \ll \mu_1$ (μ_j is the mobility of the corresponding film), the carriers are to be found mainly in the first film. Then the conductivity in a weak longitudinal electric field is determined by the first film. But if the electric field is high enough for some carriers to pass into the second (third, etc.) subband where the condition $A_2 \gg 1$ ($A_3 \gg 1$ etc.) is not satisfied, a negative conductivity may develop. To make an estimate, consider a simple heterostructure model, where the GF's are calculated near of the band edges as follows:

$$G_1 = \frac{im_1}{k_1}, \quad k_1 = \sqrt{2m_1 E}; \quad G_2 = \frac{im_2}{k_2}, \quad k_2 = \sqrt{2m_2(E - U_0)}.$$

Here m_1 and m_2 are the electron effective masses in the relevant crystals and U_0 is the energy difference between the edges of the conduction bands. Then (4) takes the form

$$\frac{1}{x} \operatorname{tg} x + \alpha(x^2 - \xi^2)^{-1/2} \operatorname{tg} a(x^2 - \xi^2)^{1/2} = 0, \quad (5)$$

where

$$x = \sqrt{2m_1 E} d_1, \quad \xi = \sqrt{2m_1 U_0} d_1, \quad \alpha = \sqrt{\frac{m_2}{m_1}}, \quad a = \alpha \frac{d_2}{d_1}$$

and the ratio of the densities of states (3) becomes

$$A = \frac{x^2 - \xi^2}{xx^2} \frac{1 + \operatorname{tg}^2 x - x^{-1} \operatorname{tg} x}{1 + \operatorname{tg}^2 a(x^2 - \xi^2)^{1/2} - a^{-1}(x^2 - \xi^2)^{-1/2} \operatorname{tg} a(x^2 - \xi^2)^{1/2}}. \quad (6)$$

A numerical calculation with $U_0 \approx 0.4$ eV, $\alpha = 2.7$, $d_1 = 100$ Å, $d_2 = 200$ Å (heterostructure p-GaSb-n-AlSb) gives now

$$E_1 = 0.04 \text{ eV}, \quad E_2 = 0.187 \text{ eV}, \quad E_3 = 0.46 \text{ eV}, \\ A_1 = 87, \quad A_2 = 34, \quad A_3 = 0.7.$$

Finally for the negative differential conductivity to appear the longitudinal electric field must exceed $\varepsilon = 4$ kV/cm.

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