SUBBAND STATES IN INVERSION LAYERS FROM SINGLE AND MULTIPLE BAND CALCULATIONS

F. Malcher, A. Ziegler, U. Rössler, G. Lommer

JOURNAL DE PHYSIQUE
Colloque C5, supplément au n°11, Tome 48, novembre 1987

SUBBAND STATES IN INVERSION LAYERS FROM SINGLE AND MULTIPLE BAND CALCULATIONS

F. MALCHER, A. ZIEGLER, U. RÖSSLER and G. LOMMER

Institut für Theoretische Physik, Universität Regensburg, D-8400 Regensburg, F.R.G.

Nous présentons des calculs self-consistants de sous-bandes pour des d'inversion sur InSb et HgCdTe en utilisant un modèle à bandes simple (2x2) et un modèle à bandes multiples (8x8). Les séparations des sous-bandes et les énergies de Fermi obtenues sont indepéndantes du modèle.

Selfconsistent subband calculations for inversion layers on InSb and HgCdTe are performed using a single (2x2) and a multiple band (8x8) model. We obtain subband separations and Fermi energies that are independent of the models.

1. Introduction

Subband states in inversion layers are influenced by the bulk band structure and the interface potential. The former is considered in the kinetic energy operator of the subband problem, whereas the potential follows for given doping profile and electron concentration N_S from the self-consistent calculation. Different band models have been used in the past to account for the nonparabolicity of the energy bands, which is of importance, particularly, for inversion layers on narrow-gap semiconductors. The standard concept, based on the Kane model [1], is the multiple band calculation. Although it was recognized quite early [1], that a proper description of the bulk band structure of InSb requires an 8x8 model, including the Γ_6 conduction band and the spin-orbit-split Γ_8 and Γ_7 valence bands, current multiple band calculations for InSb [2, 3] neglect the split-off band and the free electron term. We present two different concepts: a single band (2x2) model including higher order terms in $\mathbf{k}$, which has been successfully applied to AlGaAs/GaAs heterostructures [4] and a recently developed multiple band (8x8) model, which takes into account the full Kane Hamiltonian [5]. Selfconsistent calculations for band parameters characteristic for InSb and $Hg_{0.8}Cd_{0.2}Te$ are performed and yield subband separations E_{10}, E_{20} and Fermi energies E_F as function of electron concentration N_S. The results of these single and multiple band calculations are almost identical for InSb and at least for the lowest subbands of HgCdTe and demonstrate i) the applicability of the single band concept to inversion layers even on narrow-gap semiconductors and ii) the importance of the split-off band and remote band contributions for quantitative studies of the subband structure of these systems.

2. The 8x8 and 2x2 models

The 8x8 model for subband calculations starts from the Kane Hamiltonian $H_{\mathrm{Kane}}(\mathbf{k})$ for the coupled Γ_6 conduction and $\Gamma_8+\Gamma_7$ spin split valence bands. By replacing $\mathbf{k} \rightarrow \mathbf{k}_{\|}, \frac{1}{i}\partial_z$, where $\hbar k_{\|}$ is the conserved momentum parallel to the interface (which is perpendicular to the z–direction) and adding the interface potential $V(z)$ in the diagonal we obtain the subband Hamiltonian:

$$H_{8\mathrm{x}8} = H_{\mathrm{Kane}}(\mathbf{k}_{\|}, \frac{1}{i}\partial_z) + V(z)\mathbf{1}_{8\mathrm{x}8} \tag{1}$$

Besides the $\mathbf{k}\cdot\mathbf{p}$ coupling between Γ_6 and $\Gamma_7+\Gamma_8$ with the momentum matrixelement $P = \frac{\hbar}{m} < S|p_z|Z >$, in the kinetic energy operator also remote band contributions can be considered. The subband eigenfunction Ψ_ν of $H_{8\mathrm{x}8}$ is an eight-component spinor with envelope functions $f_i(\nu, \mathbf{k}_{\|}, z) \quad i = 1,\ldots,8$ for the eight bands. The interface potential is obtained by integrating Poisson's equation for the charge distribution

$$\rho(z) = -e\sum_{\substack{\nu\mathbf{k}_{\|}\\ \mathrm{occ.}}}\sum_{i=1}^{8}|f_i(\nu, \mathbf{k}_{\|}, z)|^2 - eN_A, \qquad 0 < z < z_d \tag{2}$$

where N_A is the volume concentration of acceptors and z_d the depletion length. $V(z)$ and z_d have to be determined in a self-consistent iteration procedure. The numerical treatment of this problem by using the concept of local solutions will be presented elsewhere [5].

The 2x2 model [4] is based on a reduction of an extended Kane model to a 2x2 conduction band Hamiltonian, which includes nonparabolicity from $\mathbf{k}\cdot\mathbf{p}$ coupling of Γ_6 with $\Gamma_7+\Gamma_8$ and remote bands by terms of higher order in the electron momentum $\mathbf{k}$. The corresponding subband Hamiltonian is again obtained by replacing $\mathbf{k} \rightarrow \mathbf{k}_{\|}, \frac{1}{i}\partial_z$ and adding the interface potential in the diagonal, which is to be calculated self-consistently from the charge distribution of occupied states and acceptors.

3. Results and discussion

For comparison of the 2x2 and 8x8 models we present first calculations for n-inversion channels on p-type material with parameters, characteristic for InSb and $Hg_{0.8}Cd_{0.2}Te$, without remote band contributions (for details see [6]). Fig. 1 shows the obtained subband separation E_{10}, E_{20} and Fermi energy E_F versus N_S. It turns out, that the results for E_{10} and E_F are almost identical, whereas E_{20} differs due to different effective masses at the subband bottom, which enter in the densisty of states and are automatically included in the 8x8 but not in the 2x2 model. These results demonstrate the capability of the 2x2 model to describe subband states at least of the lowest subband even in narrow-gap systems and allows much easier than in the 8x8 model calculations of subband Landau levels [7], which are of interest for interpreting new experimental CR and ESR data [8].

The omission of the split-off band and of the free electron term shifts the calculated energy-separations to lower values (Fig. 2). These results correspond to the frequently used 6x6 model [2, 3]. By renormalizing the momentum matrixelement P in order to get the same band edge mass as before, these shifts can be removed only partially as the conduction band dispersion remains different in the 6x6 and 8x8 model. Therefore only calculations including these terms

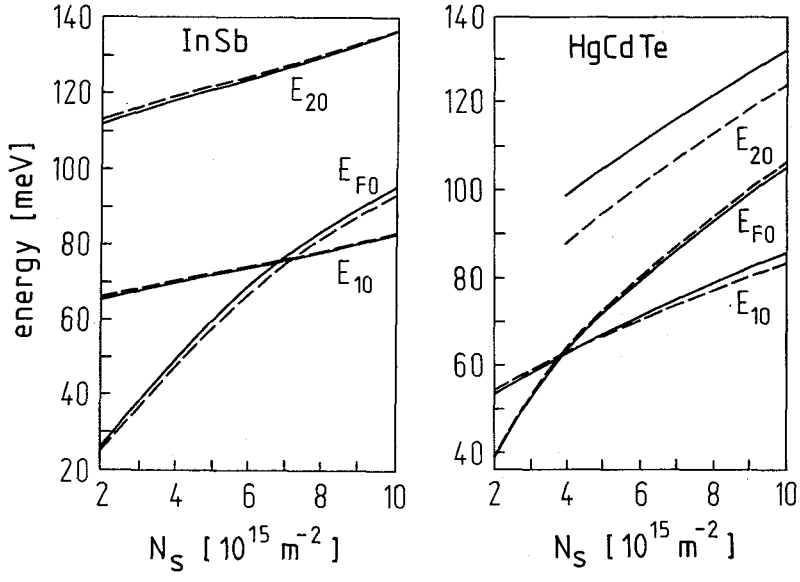

Fig. 1. Selfconsistent subband separations E_{10}, E_{20} and Fermi energy E_F obtained from the 8x8 model (solid lines) and the 2x2 model (dashed lines) versus N_S for InSb (left part) and $Hg_{0.8}Cd_{0.2}Te$ (right part), both for an acceptor concentration $N_A = 5 \cdot 10^{22}$ m^{-3}.

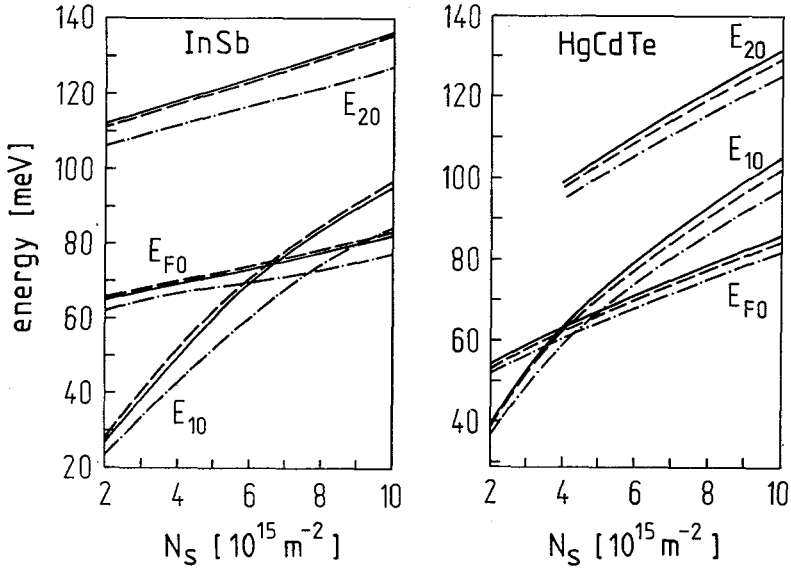

Fig. 2. Comparison of the subband separations E_{10}, E_{20} and Fermi energy E_F versus N_S calculated from the 8x8 model including remote band contributions (dashed lines), without remote bands (solid lines, see Fig. 1) and neglecting also spin-split-off band and free electron term (dashed and dotted lines) for an acceptor concentration $N_A = 5 \cdot 10^{22}$ m^{-3}.

will lead to quantitative correct results for the subband structure on narrow-gap semiconductors. The influence of remote band contributions is also shown in Fig. 2. It is stronger for HgCdTe than for InSb, as expected due to the narrower gap, and need to be considered in analyses of experiments on HgCdTe.

In conclusion, subband separations and Fermi energies from single and multiple band calculations for n-inversion layers yield identical results for InSb and even for HgCdTe for the lowest subband, if the same conduction band dispersion is used. This can be done as well in a 2x2 single band as in a 8x8 multiple band model.

References

[1] E. O. Kane, J. Phys. Chem. Solids **1** 249 (1956)
[2] Y. Takada, K. Arai, N. Uchimura, Y. Uemura J. Phys. Soc. Japan **49** 1851 (1980)
[3] G. E. Marques, L. J. Sham, Surf Sci **113** 131 (1982)
[4] F. Malcher, G. Lommer, U.Rössler, Supperlattices & Microstructures **2** 267 (1986)
[5] A. Ziegler, to be published
[6] F. Malcher, I.Nachev, A. Ziegler, U. Rössler, to be published in Zeitschrift für Physik **B**
[7] F. Malcher, G. Lommer, U. Rössler, Proc. 18th Int. Conf. Physics Semiconductors, Stockholm 1986, ed O. Engström (World Scientific) p. 493
[8] U.Merkt, M.Horst, T.Evelbauer, J.P.Kotthaus, Phys. Rev.**B 34**, 7234 (1986)