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Shallow acceptors in strained Ge/GeSi heterostructures with wide quantum wells

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Abstract. Energy spectra of shallow acceptors in uniaxially stretched Ge were calculated by variational technique. The results were used for the interpretation of the observed far infrared photoconductivity spectra of strained Ge/GeSi heterostructures with wide quantum wells.

Introduction

The paper deals with shallow acceptors in wide quantum wells (QWs) in germanium layers in strained $Ge/Ge_{1-x}Si_x$ heterostructures grown on Ge(111) substrates. The deformation of Ge layers is equivalent to hydrostatic compression and uniaxial tension along the growth direction. The uniaxial part of the deformation splits the light and heavy hole subbands [1]. In wide QWs (with respect to a typical Bohr radius of acceptors) in Ge/GeSi heterostructures shallow acceptor are affected mainly by the strain rather than by the size quantization. Therefore at zero approximation the shallow acceptors in Ge/GeSi heterostructures can be treated as impurities in bulk Ge subjected to the uniaxial tension. Shallow acceptors in uniaxially compressed Ge were theoretically investigated in [1, 2]. It was shown that the compression results in the splitting of four-fold degenerated ground and excited states into pairs of two-fold degenerated states. In the present paper the variational calculations of shallow acceptors in uniaxially stretched along (111) direction Ge have been carried out using the effective mass approximation. The results are shown to be in a good agreement with the observed spectra of far IR (FIR) photoconductivity of p-type Ge/GeSi heterostructures.

1 Theory

In the case of uniaxial deformation the Hamiltonian in the envelope function equation for the valence band in Ge is the sum of 4×4 matrix Luttinger Hamiltonian [3] and the deformation term [1]. This Hamiltonian describes light and heavy hole subbands and the envelope wave function $F_j(r)$ $(j = 1-4)$ is four-dimensional vector. Eigenvalues of the envelope function equation with the Coulomb term in the Hamiltonian for the shallow acceptor in uniaxially stretched Ge were found by variational method in the manner similar to that used for the calculation of acceptor spectra in unstrained Ge [4]. Trial wave functions for variational calculation of acceptor spectra in strained Ge were

chose by similar [4] procedure. Trial wave functions were taken in the form

$$F_j(r,\theta,\varphi) = \sum_l r^l \exp\left(-\frac{r}{r_l}\sqrt{\sin^2\theta + q^2\cos^2\theta}\right)\sum_{m=-l}^{l} c_{lm}^j \sin^m\theta \frac{d^{|m|}P_l(q\cos\theta)e^{im\varphi}}{d(q\cos\theta)^{|m|}}$$

where $c_{l,m}^j$, r_l and q (parameter of anisotropy) are variational parameters, P_l is the Legendre polynomials of $q\cos\theta$. Here $l = 0, 2$ for the ground state and $l = 1, 3$ for the lowest excited states, z axis is chosen along the tension direction. The variational procedure can be simplified significantly by the reducing of the number of variational parameters taking into account the crystal symmetry. In uniaxially stretched Ge the double point symmetry group D_{3d} corresponds to the center of Brillouin zone (Γ-point). The same group corresponds to the point L in unstressed Ge. Therefore wave function of acceptor should be transformed by additional irreducible representations of double group in point L. There are six additional irreducible representation of group D_{3d}: $L_4^{\pm}$, $L_5^{\pm}$, $L_6^{\pm}$. One-dimensional representations $L_4^{\pm}$ and $L_5^{\pm}$ are complex conjugated; therefore they should be considered as one two-dimensional representation. Representation $L_6^{\pm}$ is two-dimensional. Wave function of the ground acceptor state transforms according to the irreducible representations which correspond to the top of valence band: $L_{4,5}^{+}$ (heavy holes) and L_6^{+} (light holes). Dipole optical transitions from the ground state are allowed only into odd (respect to the inversion) excited states. The lowest odd excited states are p-like states. Therefore their wave functions should transform according to the irreducible representations $L_{4,5}^{-}$ and L_6^{-}.

The results of the calculations of the acceptor binding energies for the ground and the lowest excited states are plotted in Fig.1 as a function of the deformation. It is clearly seen that the deformation splits the ground state into $L_{4,5}^{+}$ and L_6^{+} levels; the last one rapidly shifts to the continuum with the deformation. Binding energies of few

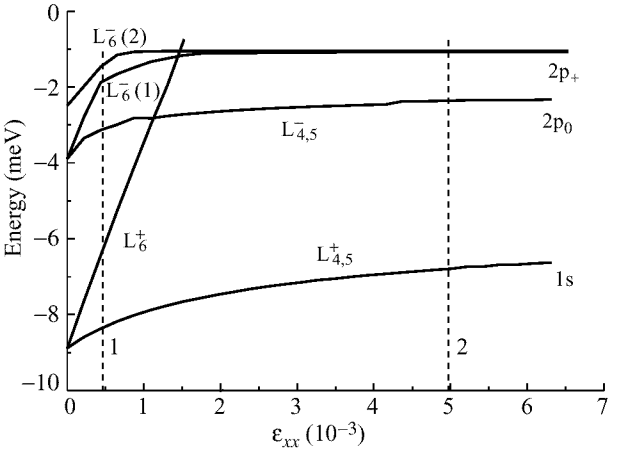

Fig 1. Binding energies of the ground and the lowest excited states of shallow acceptor in uniaxially stretched Ge versus the component ε_{xx} of the deformation tensor (all other components are proportional to ε_{xx}). Vertical dashed line 1 and 2 indicate the deformation value for the sample # 309 and the "effective" deformation value for the sample #306.

lowest p-like excited states were calculated: $L^-_{4,5}$, $L^-_6(1,2)$. At high stress the influence of the split off light hole subband may be neglected and the acceptor spectra may be calculated as in the case of simple anisotropic band [5]. In Fig. 1 one can see that with the increase of the deformation the binding energies tend to the asymptotic values corresponding to $1s$, $2p_0$ and $2p_\pm$ levels of the simple anisotropic model [5]. In another limit $\varepsilon \to 0$ the results obtained are in a good agreement with those calculated for the unstressed Ge [3].

2 Experiment and discussion

The results of the calculations performed allow to interpret the experimental spectra of impurity FIR photoconductivity of Ge/GeSi heterostructures. The spectra were measured by using BOMEM DA3.36 FT spectrometer [6]. Fig. 2 represents photoconductivity spectra of two undoped sample # 306,# 309 (with residual acceptor impurities) and of the sample # 379 with boron doped QWs.

Photoconductivity spectrum of the sample #309 (Fig. 2a) with thick Ge layers consists of the line at $\hbar\omega \approx 5.3$ meV and the broad band at $\hbar\omega = 7-10$ meV. The line at $\hbar\omega \approx 5.3$ meV corresponds to the transition between ground state $L^+_{4,5}$ and the first excited state $L^-_{4,5}$ (Fig. 1). The energy separation between $L^+_{4,5}$ and $L^-_6(1)$ states corresponds to $\hbar\omega = 7$ meV that corresponds fairly well to beginning of short-wavelength photoconductivity band in the spectrum in Fig. 2a. At higher frequencies the photoconductivity may be explained by transitions to higher excited states and in the continuum.

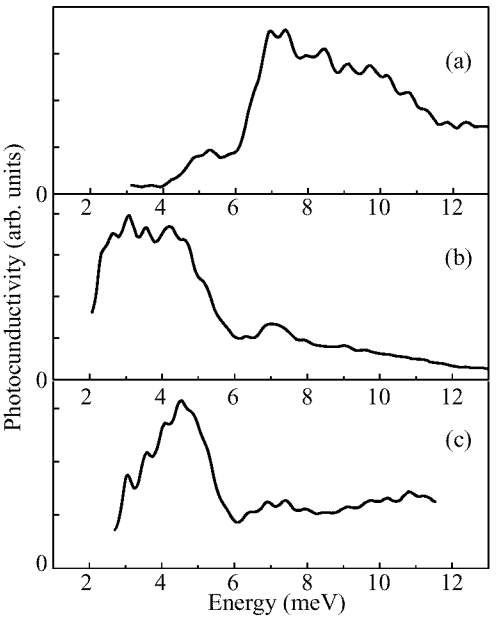

Fig 2. Impurity photoconductivity spectra of Ge/GeSi MQW heterostructures at $T = 4.2$ K; a: # 309 ($d_{QW} = 800$ Å), b: # 306 ($d_{QW} = 200$ Å), c: # 379 ($d_{QW} = 200$ Å).

According to the results of the calculations the typical wave function extension (Bohr radius) in direction of deformation is about 40 Å. Therefore the effect of size quantization on the acceptor spectrum is more pronounced in the samples # 306, 379 with narrower QWs. The energy gap between light and heavy hole subbands in these samples is 30–40 meV (cf. with 3 meV in # 309). This effect was taken into account by introducing the effective deformation which corresponds to the total splitting of the subbands (vertical line 2 in Fig. 1). This approach allows the qualitative description of the observed spectra (Fig. 2b,c). The position of the spectral line $\hbar\omega \approx 6.9$ meV is in a good agreement with the energy separation between the ground state $L^{+}_{4,5}$ and the continuum for the sample #306 (Fig. 1). The strongest line in the spectra in Fig. 2b,c should be naturally attributed to the transition between the ground state and excited state which turns into $2P_{\pm}$ level in the model of simple anisotropy band [5]. This transition should correspond to the frequency $\hbar\omega \approx 5.5$ meV. However the short-wavelength edge of the strongest photoconductivity band in Fig. 2b,c corresponds to a little bit lower frequency $\hbar\omega \approx 5$ meV. This indicates the necessity to consider the confinement effects on the excited impurity states more correctly.

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