Subband energies in *n*-channel inversion layers on (111) Ge

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The subband structure of electrons in a space-charge layer on (111) Ge has been evaluated self-consistently in the local-density-functional formalism. The results show that several subbands are filled at readily accessible inversion-layer densities and thus support the interpretation of experiments performed in this material.

I. INTRODUCTION

In a metal-insulator-semiconductor structure an inversion layer can be formed near the insulator-semiconductor surface when a voltage is applied across the insulator. This space-charge layer has now been studied in many different semiconductors.[1] Most widely studied and best understood is Si, in particular *n*-channel inversion layers on (100) surfaces. In the latter case the effective-mass approximation works very well. From a theoretical point of view an *n*-channel inversion layer on (111) Ge is expected to be very similar, but only recently have experimental investigations given good results on the subband structure.[2] It is thus of interest to carry out a theoretical calculation of the subband energies and compare it with the experiment. The most interesting qualitative difference between Si and Ge is that whereas it is difficult to occupy more than one subband in Si at low temperatures, several subbands are readily filled in Ge.

II. THEORY

The effective-mass approximation applied to (111) Ge surfaces was described by Stern and Howard[3]: The valley which has its longitudinal mass perpendicular to the surface gives rise to one ladder of subbands denoted 0,1,2, etc., whereas the other three valleys give rise to another, higher lying ladder of subbands 0′, 1′, 2′, etc. In Table I the parameters relevant for our calculation are listed and, in analogy with the theory for Si,[4] the subband energies E_i and envelope wave functions ζ_i are described by the Schrödinger equations

$$\left(-\frac{\hbar^2}{2m_3}\frac{d^2}{dz^2}+V_{\rm dep}+V_H+V_{\rm im}+V_{xc}\right)\zeta_i(z)=E_i\zeta_i(z)\ ,$$

$$\left(-\frac{\hbar^2}{2m_3'}\frac{d^2}{dz^2}+V_{\rm dep}+V_H+V_{\rm im}+V_{xc}'\right)\zeta_{i'}(z)=E_{i'}\zeta_{i'}(z)\ ,$$

where $V_{\rm dep}(z)=e^2N_{\rm dep}z/\epsilon_s$ is the depletion potential, $V_H(z)$ is the Hartree potential from the electrons determined by Poisson's equation, and

$$V_{\rm im}(z)=(\epsilon_s-\epsilon_i)e^2/16\pi\epsilon_s(\epsilon_s+\epsilon_i)z$$

is the image potential. The effects of exchange and correlation are taken into account through the local exchange-correlation potentials V_{xc} and V_{xc}'. They depend on the local densities of electrons in the unprimed $n(z)$ and primed $n'(z)$ subband systems and directly on z because of the different permittivities of the insulator and Ge. z is in the direction perpendicular to the surface, and the origin is at the interface.

A self-consistent solution is then found by filling all states below the Fermi energy E_F keeping the total density of electrons N in the inversion layer constant as expressed by the following equations:

$$N=\sum_i N_i+\sum_{i'}N_{i'}\ ,$$

$$N_i=(E_F-E_i)\Theta(E_F-E_i)\,n_v m_d/\pi\hbar^2\ ,$$

$$N_{i'}=(E_F-E_{i'})\Theta(E_F-E_{i'})\,n_v' m_d^{i}/\pi\hbar^2\ ,$$

$$n(z)=\sum_i N_i|\zeta_i(z)|^2\ ,$$

$$n'(z)=\sum_{i'}N_{i'}|\zeta_{i'}(z)|^2\ ,$$

and iterating until the potentials and density distributions have converged.

For the exchange-correlation potentials[5] we have used the exchange-correlation contributions to the chemical potential of a homogeneous gas of density $n+n'$. The electrons have 2 spin and 4 valley degrees of freedom. Thus the valley which has its longitudinal mass perpendicular to the surface is filled with n electrons, and V_{xc} is the exchange-correlation contribution to the chemical potential of these electrons, while the other three valleys contain each $\frac{1}{3}n'$ electrons and V_{xc}' is the exchange-correlation contribution to the chemical potential of those electrons. It is assumed that intervalley exchange processes can be neglected compared with intravalley processes because of the large momentum transfer required, so the procedure outlined here is a natural extension of the spin-density-functional formalism.[6] Technically

TABLE I. Notation and values of parameters used in the calculation. ϵ_0 is the permittivity of vacuum and m_0 the free-electron mass.

Permittivity of semiconductor	ϵ_s		$16\ \epsilon_0$
Permittivity of insulator	ϵ_i		$3\ \epsilon_0$
Longitudinal effective mass of Ge	m_l		$1.6\ m_0$
Transverse effective mass of Ge	m_t		$0.08\ m_0$
Effective mass perpendicular to interface	m_3	m_l	$1.6\ m_0$
	m_3'	$9m_tm_l/(m_t+8m_l)$	$0.089\ m_0$
Subband density of states mass	m_d	m_t	$0.08\ m_0$
	m_d'	$[m_t(m_t+8m_l)/9]^{1/2}$	$0.338\ m_0$
Subband valley degeneracy	n_v		1
	n_v'		3
Depletion layer density	N_{depl}		$2.5\times10^{10}\ \text{cm}^{-2}$

we have calculated these potentials in the plasmon-pole approximation[7] with an electron-electron interaction modified as suggested by Ando[4] to describe approximately the effect of the different permittivities of insulator and semiconductor. Furthermore, the anisotropy of the mass was neglected, as is usual practice in electron-hole drop calculations.[8] For the results presented here the conductivity mass $3m_c^{-1}=2m_t^{-1}+m_l^{-1}$ was used; the results do not change significantly, if the density-of-states mass $m_{\text{DOS}}^3=m_t^2m_l$ is used.

III. RESULTS AND DISCUSSION

In Fig. 1 we show the subband energies and the Fermi energy as functions of inversion-layer density. Compared with the results[4] in (100) Si two features are significantly different. Firstly, the density of states in the unprimed subbands is smaller because of the smaller transverse mass of Ge and the lack of valley degeneracy. This means that the Fermi energy increases much faster with inversion-layer density, so that the first excited subband starts to be occupied below $N_{\text{inv}}=3\times10^{11}\ \text{cm}^{-2}$ and the second below $10^{12}\ \text{cm}^{-2}$. Secondly, the large mass anisotropy and thereby the smaller value of m_3' pushes the 0′ subband higher up in energy: In Si the first excited and the 0′ subband are very close in energy. Here E_3 and $E_{0'}$ lie very close. In fact $E_3>E_{0'}$ below $10^{12}\ \text{cm}^{-2}$, $E_3<E_{0'}$ for $10^{12}\ \text{cm}^{-2}<N_{\text{inv}}<2.4\times10^{12}\ \text{cm}^{-2}$, and $E_3>E_{0'}$, for larger densities, but they lie so close that for clarity E_3 has been left out of the drawing. In general the subband separations in the unprimed set are smaller than in Si because of the larger longitudinal mass of Ge.

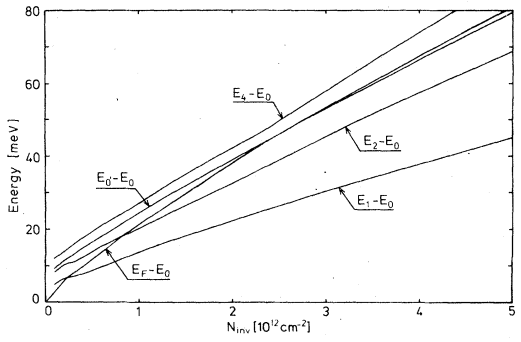

FIG. 1. Subband energies and Fermi energy as functions of inversion-layer density. E_3 is very close to $E_{0'}$.

In Fig. 2 is shown the number of electrons in each subband as a function of total inversion-layer density. Clearly a substantial fraction of the electrons goes into higher subbands at easily accesible densities. Quantitatively it is remarkable that in each subband the number of electrons increases very linearly with N_{inv} except for the change in slope whenever a new subband starts being occupied.

Also shown are the subband occupation numbers determined experimentally from Shubnikov–de Haas oscillations.[2] Certainly the calculation supports the interpretation that the oscillations originate from sub-

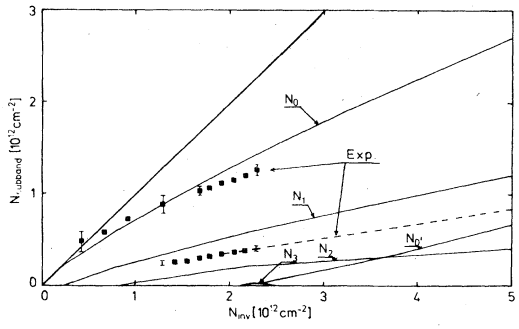

FIG. 2. Calculated population of subbands as a function of total inversion-layer density. Also shown are the measurements by Binder *et al.*, Ref. 2. Single points: Lacquer insulator. Broken line: Mylar-foil insulator.

band states 0 and 1. Quantitatively the agreement is not perfect, however. The main problem is that, even if one allows for some uncertainty in determining the threshold voltage, not all the carriers that are induced are seen in the Shubikov–de Haas oscillations, and it is not known where the remaining electrons go. The ratio N_0/N_1 is roughly constant over a fairly large range around $N_{inv} = 2 \times 10^{12}$ cm^{-2}. Experimentally $N_0/N_1 \cong 3.2$ is significantly larger than the theoretical value of 2.4. This shows that the remaining carriers cannot simply be trapped in strongly localized surface or insulator states: That would only reduce the actual number of electrons in the inversion layer and not affect the inversion-layer potential in any other way. Furthermore, it is unlikely that they are in the second excited subband because their number is so large and their mobility expected to be even better than in subband 1 that they should be observable in the Shubnikov–de Haas experiment. The best suggestion is probably that the 0′ subband lies lower than calculated in the present theory. Binder *et al.*[2] have argued that the large density of states in that subband makes observation of Shubnikov–de Haas oscillations from the remaining carriers improbable, even if they all go into that subband. It is not unexpected that our theory should predict a too large $E_{0'}$, since it is assumed that the energy barrier between insulator and semiconductor is abrupt and infinitely high, so that the wave functions are equal to zero at the interface. Stern[9] has investigated what happens to the subband energies in Si, if the energy barrier is finite and if the barrier is not abrupt but increases gradually over a transition region, so that the wave functions penetrate into the insulator. The strongest effect found was indeed a reduction of $E_{0'} - E_0$ relative to the infinite barrier case and a much smaller reduction within each subband ladder. The trends of his calculation all indicate that the effect should be even stronger for the system discussed here: Basically the difference between the primed and unprimed subbands originates from the condition that the probability current or $m_3^{-1}\, d\zeta/dz$ be continuous at the interface. Since the mass anisotropy m_3/m_3' is almost four times larger in Ge than in (100) Si, the reduction of $E_{0'}$ is enhanced. Also it is certain that the interface is much less perfect than the Si-SiO_2 interface. This corresponds to a larger transition region and thereby a stronger reduction. In Stern's model the reduction of $E_{0'} - E_0$ is characteristically between 5 and 15 meV, so it is quite conceivable that $E_{0'}$ is moved down to or below E_2 in our case. The low mobility of the electrons in the lowest subband is also consistent with a strong effect of the transition region at the interface. However, in view of the very limited knowledge of the properties of the insulator and the real interface we have not attempted to model this effect for the Ge space-charge layer.

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