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Many-body effects on the subband structure of n-type surface space-charge layers in InP

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The effects of both the direct and the polar LO-phonon mediated electron-electron interactions are included in a calculation of the many-body effects on the subband structure of InP. The results show that the effects of exchange and correlation among surface electrons are not negligible. The dominant contribution to electronic self-energy correction comes from the direct electron-electron interaction. The threshold densities of higher-subband occupancy are determined and compared with existing models and experiments.

In recent years there has been an increasing interest in the study of electronic properties of surface space-charge layers on a polar semiconductor,[1,2] especially in the III-V compounds.[3–6] Contrary to the case of elemental semiconductor surface space-charge layers, the exchange-correlation effects seemed small in the accumulation region of the InP layers. The main reason for this could be attributed to the relative smallness of the parameter r_s (or the small effective mass) of InP.[5] The subband structures of InP are surprisingly in good agreement in the Hartree[5] and density-functional approximations.[7]

A proper theory of the subband structure for a polar semiconductor should include the electron-electron interactions, both the direct Coulomb interaction, and the phonon mediated interaction. The contribution of the latter interaction is expected to become more significant as one goes to a more polar material such as InP. Kawamoto, Bloss, and Quinn[3] have studied the subband structure of InP, including the exchange-correlation effects, in the region of high depletion-charge concentration. The purpose of the present work is to emphasize the importance of the many-body effects in determining the threshold density for higher-subband occupancy in InP surface space-charge layers in an accumulation region. The electronic subband structure in a surface space-charge layer of InP is calculated in the framework of the energy-functional perturbation approach.[8,9] The effects of both the direct and the polar LO-phonon mediated electron-electron interactions are included in the calculation.

Bulk InP has a direct band gap with a single conduction-band minimum at the Γ point. If one considers only the nondegenerate regime of surface electron concentration, the conduction-band minimum can be approximated as a parabolic one. Due to the relatively large band gap [~1.42 eV (Ref. 10)], the effect of coupling between the conduction and the valence bands is not expected to be significant in the case of InP. Also, there is no problem of multiple-valley occupancy, as in Si.[8] Therefore, if one uses the effective-mass approximation,[11] the single-particle calculation of InP is much simpler than other cases of narrow band gap or multivalley structure. We employ the effective-mass approximation in the present calculation because of this large band gap in InP and the resulting parabolic–conduction-band minimum.

The calculation begins by solving the single-particle problem within the effective-mass approximation. Variational solutions to the Kohn-Sham equation are used as the basis in the calculation of the self-energy correction to the subband energy.[8,9] The one-dimensional effective potential $V_{\mathrm{eff}}(z)$ consists of the usual electrostatic potential plus an exchange-correlation potential v_{xc}, which is a functional of the local electron density $n(z)$. Here Z is normal to the interface $(z=0)$. One should note that the use of the static dielectric constant ϵ_0 in the effective potential $V_{\mathrm{eff}}(z)$ is consistent with (4) below.[3] One can take a number of different approximate expressions[12] for the exchange-correlation potential v_{xc}, which take account of the major effects of exchange and correlation between electrons. In this calculation, v_{xc} is taken to be of the form[8,9]

$$v_{\mathrm{xc}}\{n(z)\} = -\alpha n^{1/3}(z)[1+Cn_v^{2/3}n^{-1/6}(z)] \ , \tag{1}$$

where $\alpha=(e^2/2\epsilon_0)(24/\pi n_v)^{1/3}$ is the usual coefficient of the exchange potential, n_v is the valley occupancy ($n_v=1$ for InP), and C is a correlation parameter to be adjusted later in the calculation. The term involving the parameter C in (1) is an approximation to the correlation contribution to a local exchange-correlation potential. In order to obtain the subband self-energy correlation we introduce the electron-electron interaction $V^{e\text{-}e}(\vec{r}-\vec{r}\,';z,z')$, where $\vec{r}=(x,y)$. In the case of a polar semiconductor such as InP, $V^{e\text{-}e}$ should include a contribution from a phonon mediated electron-electron interaction $V^{e\text{-ph}}$, as well as a bare Coulomb interaction V^{Coul}:

$$V^{e\text{-}e} = V^{\mathrm{Coul}} + V^{e\text{-ph}} \ . \tag{2}$$

It is not a simple task to include the term $V^{e\text{-ph}}$ rigorously in the calculation. However, if we assume that electrons couple dominantly with dispersionless longitudinal-optical phonons, the calculation becomes much simpler.[13]

The difference H' between the full electron-electron interaction and the single-particle approximation is treated as a perturbation[9]:

$$\begin{aligned} H' = \tfrac{1}{2}\int\int d\vec{x}\,d\vec{x}\,'\psi^\dagger(\vec{x})\psi^\dagger(\vec{x}\,')\,V^{e\text{-}e}(\vec{x},\vec{x}\,')\psi(\vec{x})\psi(\vec{x}\,') \\ -\int d\vec{x}[V_H(\vec{x})+v_{\mathrm{xc}}(\vec{x})]\psi^\dagger(\vec{x})\psi(\vec{x}) \ , \end{aligned} \tag{3}$$

where $\vec{x}=(\vec{r},z)$ and $\psi^\dagger(\vec{x})$ and $\psi(\vec{x})$ are field operators. The Hartree potential is given by

$$V_H(\vec{x}) = \int d\vec{x}\,'\,V^{e\text{-}e}(\vec{x},\vec{x}\,')n(\vec{x}\,') \ , \tag{4}$$

where the density $n(\vec{x})$ is defined by

$$n(\vec{x}) = \langle\psi^\dagger(\vec{x})\Psi(\vec{x})\rangle \ . \tag{5}$$

The dynamic screening of surface layer electrons could be included through the use of the plasmon-pole approximation,[14] in which one approximates the terms beyond the exchange (static screening) term by a coupling to a single effective plasmon. We note that the so-called tadpole diagram is canceled exactly by the electrostatic term (the second term) in H'. The parameter C is varied until the ground subband self-energy correction due to H' for a particle at the Fermi surface becomes zero:

$$\Sigma_{00}(k_f,\epsilon_0(k_f),C)\equiv 0 \;, \qquad (6)$$

where $\epsilon_n(k)$ is the excitation energy. Σ_{00} vanishes by choice of the parameter C, but Σ_{nn} is finite for $n\neq 0$. Here,

$$\epsilon_n(k)=E_n(k)-\mu+\Sigma_{nn}(k,\epsilon_n(k)) \;, \qquad (7)$$

where $E_n(k)$ are the single-particle energies and μ is the Fermi level. In Fig. 1, we give the energy separations $\tilde{E}_{n0}$ for the lowest three subbands as a function of surface electron concentration in a relatively low surface density regime. We have neglected the effect of intersubband mixing, which turned out to be small in this calculation. The physical quantities in Table I are used to obtain the results shown in Fig. 1. We have also shown the results (dotted line) E^H_{n0} of the Hartree approximation. The enhancement in $\tilde{E}_{n0}$ from E^H_{n0} is mainly due to the large exchange energy of the ground subband (compared with those of the higher subbands). Some of the reported E^H_{10} results are indicated. In Ref. 5, the Hartree calculation was done at finite temperatures with the use of variational wave functions and the high-frequency dielectric constant ϵ_∞ in V_{eff}. In this latter calculation, the first excited subband appeared to be already occupied at an electron concentration of $N_x \lesssim 3\times10^{11}$ cm^{-2}. A local density-functional calculation[7] gives E_{10}, which are very close to E^H_{10} of Ref. 5. In fact, the magnitude of the subband separations strongly depends upon the choice of the parameters (such as ϵ_0 or ϵ_∞) in the calculation.

TABLE I. Physical quantities for InP surface space-charge layers.

Electron effective mass	$m^*=0.0803m_e$
LO phonon energy	$\hbar\omega_{\text{LO}}=42.8$ meV
Static dielectric constant	$\epsilon_0=12.6$
Optical dielectric constant	$\epsilon_\infty=9.6$
Insulator dielectric constant	$\epsilon_{0x}=3.9$
Depletion layer concentration	$N_{\text{depl}}=10^{10}$ cm^{-2}

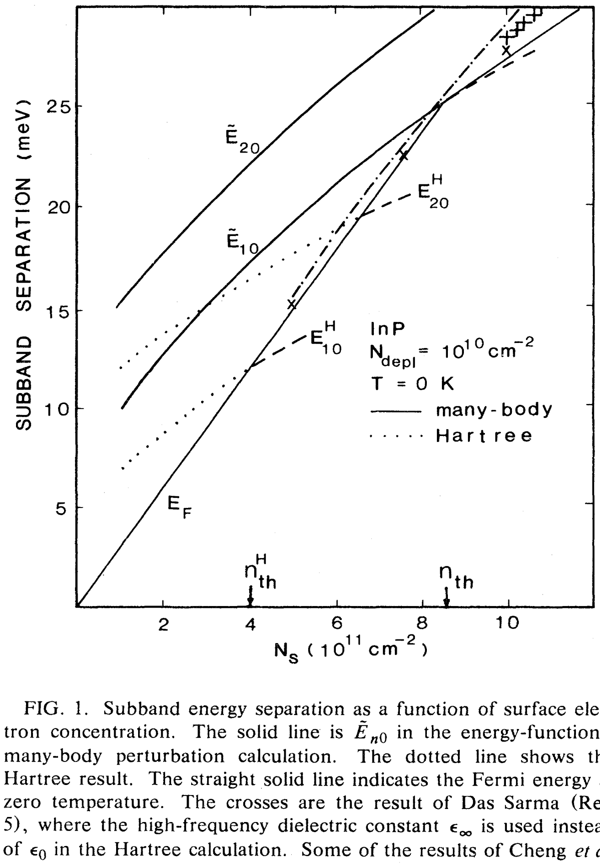

FIG. 1. Subband energy separation as a function of surface electron concentration. The solid line is $\tilde{E}_{n0}$ in the energy-functional many-body perturbation calculation. The dotted line shows the Hartree result. The straight solid line indicates the Fermi energy at zero temperature. The crosses are the result of Das Sarma (Ref. 5), where the high-frequency dielectric constant ϵ_∞ is used instead of ϵ_0 in the Hartree calculation. Some of the results of Cheng *et al.* (Ref. 6) and Tränkle (Ref. 7) are also shown by the pluses and the dot-dashed line, respectively, near n_{th}. The threshold densities at which the higher subbands begin to become occupied are also indicated both in the Hartree (n^H_{th}) and many-body (n_{th}) calculations. The input parameters employed in Ref. 7 are not available for direct comparison with other results.

The variational scheme, in general, overestimates the energies through the use of approximate wave functions for the subbands. If the exchange and correlation have a significant effect, the Hartree results, which are used as a basis set in the conventional many-body calculation, may give a less physical result due to a large self-energy correction to the quasiparticle energies.[3] The dominant contribution to self-energy comes from the electron-electron interaction. The contribution of the electron-phonon coupling through the polar LO modes is also included in the quasiparticle energy. The electron-phonon coupling turns out to give less self-energy correction for the higher subbands and hence reduces the overall subband separations by a few meV. The threshold electron concentration n_{th}, at which the higher subband starts to be occupied, is also in a more reasonable range ($n_{\text{th}}\gtrsim 0.8\times10^{12}$ cm^{-2}) in our calculation compared with the Hartree result ($n_{\text{th}}\lesssim 0.3\times10^{12}$ cm^{-2}) of Ref. 5. On InP inversion layers ($N_{\text{depl}}>10^{11}$ cm^{-2}), the ground subband only is occupied until the surface electron concentration becomes very high.[3] In a recent experimental study[6] of Shubnikov-de Haas oscillations in InP, it was reported that the subband splitting $\tilde{E}_{10}$ was ~ 28 meV at $N_s\sim10^{12}$ cm^{-2} (as shown in Fig. 1) and two-subband occupancy was found just above the density of 10^{12} cm^{-2}, which are in excellent agreement with our calculations.

In conclusion, we present a more complete many-body study of the electronic subband structure of an InP-surface space-charge layer within an energy-functional perturbation approach. The self-energy correction due to the coupling of an electron and a polar LO phonon reduces the overall subband separation. The effect of exchange and correlation among surface electrons is significant in the subband separation and higher subbands begin to be occupied at a surface electron concentration of $N_s\approx 8\times10^{11}$ cm^{-2}, which is in good agreement with experimental observations in InP accumulation layers.

ACKNOWLEDGMENT

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