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Modified Thomas-Fermi theory for depletion and accumulation layers in *n*-type GaAs

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A modified Thomas-Fermi approximation (TFA) developed originally for inversion layers is used to calculate electron-density profiles, the spatial dependences of the potential, surface potentials, and the energies of bound states of depletion and accumulation layers in *n*-type GaAs. Remarkable agreement with recently published results of self-consistent calculations of Ehlers and Mills [Phys. Rev. B **34**, 3939 (1986)] is achieved. All deficiencies of the conventional TFA discussed there are removed. Methodological advantages of the modified TFA are discussed.

Recently, Ehlers and Mills[1] presented self-consistent calculations of depletion- and accumulation-layer profiles in *n*-type GaAs. Accumulation layers in metal-insulator-semiconductor (MIS) systems have been investigated since the mid-1960's[2–7] but much more attention has been devoted to inversion layers.[7] Thus, especially in connection with new experiments, interest in the electronic structure of accumulation and depletion layers continues. In self-consistent solutions of the Schrödinger equation and Poisson's equation for accumulation layers, bound and mobile electron states must be included. As in other works,[2–4] Ehlers and Mills[1] fitted the self-consistent potential to an analytic form which allowed them to use a series method to obtain a single-particle bound state.

Ehlers and Mills[1] compared their results for the surface potential, the spatial variations of the potential, and the electron-density profile to results obtained from the Thomas-Fermi approximation[8] (TFA). They found "the Thomas-Fermi description rather poor for the parameter range considered." Actually the spatial dependences of band edges and densities, respectively, differ considerably not only quantitatively but also, especially in the flat-band case, qualitatively. (i) In the TFA the density exhibits generally a monotonic variation with position up to the surface and remains finite up to the surface, whereas the boundary condition for the wave function actually requires the density to decrease smoothly to zero (the small tail which leaks out into the insulator can be ignored). (ii) As a consequence of this qualitatively wrong picture for the density, the potential also becomes erroneous in the TFA and in the flat-band case qualitatively. (iii) The TFA is not capable of yielding the bound states (bottoms of two-dimensional subbands) in the accumulation case. Ehlers an Mills[1] attributed the deficiencies of the TFA in the discussion of their results to the fact that the boundary condition for the wave function is not fulfilled. But additionally they stated that the TFA assumes the de Broglie wavelength to be small compared to the screening length, an inequality satisfied nowhere in the carrier density range considered.

We wish to show that there exists a possibility of including the boundary condition for the wave functions by properly modifying the TFA [MTFA (Ref. 9)]. The application of the MTFA to depletion and accumulation layers removes the above-mentioned deficiencies of the TFA. Further advantages of the MTFA will be given at the end of this Brief Report. The MTFA was developed by us for the description of inversion layers (denoted as modified local-density approximation). The basic idea was the derivation of an analytic approximation for the density which takes into account the boundary condition for the envelope wave functions at the surface or interface (at $z=0$, the semiconductor in the half-space $z>0$) modeled by a high potential barrier. For a semiconductor with an isotropic parabolic conduction band and a position-dependent band edge $V_c(z)$ one obtains for the electron density in the conduction band, averaged over atomic dimensions[9]

$$n(z)=\frac{2N_c}{\sqrt{\pi}}\int_0^\infty d\varphi\frac{\varphi^{1/2}}{1+e^{\varphi-\kappa(z)}}\left[1-j_0\left(\frac{2z}{L}\varphi^{1/2}\right)\right],$$

$$j_0(a)=\sin a/a,\quad L=\hbar/(2m_nk_BT)^{1/2}, \tag{1}$$

$$\kappa(z)=[\mu-V_c(z)]/k_BT,\quad N_c=\frac{1}{4}\left(\frac{2m_nk_BT}{\pi\hbar^2}\right)^{3/2}.$$

m_n is the effective mass of the conduction band (GaAs: $m_n=0.069m_e$), μ is the chemical potential determined by the bulk neutrality, and k_BT is the thermal energy. The expression (1) smoothly vanishes to zero at the interface $[j_0(z\to 0)\to 1]$ as the wave functions do. For large distances $z\gg L$ from the interface $[j_0(z\to\infty)\to 0]$ (1) is reduced to the usual TFA for the density for an arbitrary degree of degeneracy. Equation (1) and its extensions to many-valley semiconductors[10] and to semiconductors with nonparabolic band structure[11] were successfully used to calculate the electronic subband structure of inversion layers.[12,13]

For the application of (1) to accumulation layers one has to be aware of the fact that (1) describes both bound and mobile electrons. This problem will be discussed in more detail in a subsequent paper.[14] With (1) one immediately can solve Poisson's equation

$$\frac{d^2V_c(z)}{dz^2}=\frac{e^2}{\epsilon\epsilon_0}[N_D^+(z)-n(z)] \tag{2}$$

numerically[12] (ϵ is the dielectric constant of the semiconductor). For the effective concentration $N_D^+(z)$ of donors as a function of the band bending, the common description[15]

$$N_D^+(z)=N_D^+\frac{1+2\exp[(\mu-V_c^b+E_B)/k_BT]}{1+2\exp\{[\mu-V_c(z)+E_B]/k_BT\}} \tag{3}$$

(where V_c^b represents the bulk potential) is used with the donor energy $E_B=6.5$ meV (Ref. 1) and the bulk effective donor concentration N_D^+. Once the potential $V_c(z)$ is obtained we can use the modified Bohr-Sommerfeld quantization formula[16]

$$\int_0^{z_i^+} dz \left[\frac{2m_n}{\hbar^2}[E_i-V_c(z)]\right]^{1/2}=\tfrac{2}{3}\,|a_i|^{3/2} \tag{4}$$

to calculate for the accumulation case the bound-state energies E_i and hence the subband $E_i+\hbar^2(k_x^2+k_y^2)/2m_n$. The a_i are the roots of the Airy function and z_i^+ the classical turning point, $V_c(z_i^+)=E_i$.

Calculations were carried out for depletion and accumulation layers in n-type GaAs at $T=300$ K. Figure 1 shows the dependence of the bound-state energies $E_i-V_c^b$ and the valence-band bending, or surface potential, $V_c(0)-V_c^b$, on the total charge

$$Q=-(\epsilon\epsilon_0/e)(dV_c/dz)\,|_{z=0} \quad (\epsilon=11.9)$$

for three different donor concentrations. Whereas the original TFA is of limited quantitative validity, most particularly in the accumulation region $Q<0$, as pointed out by Ehlers and Mills,[1] the MTFA shows a good overall agreement with the self-consistent results.[1] Of special importance is the fact that the flat-band case (the point where the potential vanishes) occurs correctly not for $Q=0$ but for a positive value of Q by virtue of the boundary condition for the wave functions which causes a deficit of electron charge. But not only this qualitative peculiarity is reproduced well by the MTFA. It is seen that there is a remarkable overall agreement. This concerns also the fact that the surface potential changes more strongly with Q than in the simple TFA. Only for the highest donor concentration in Fig. 1 do small differences to the results of Ehlers and Mills[1] occur. In Fig. 2 we show the spatial variation of the potential (the band bending) and the conduction-electron-density distribution. Both quantities are shown for three values of donor concentration and for three values of the total charge Q. The upper row for the potentials shows the good agreement of the MTFA with the full theory,[1] whereas the usual TFA provides a rather poor fit.[1] The electron density in the TFA exhibits a monotonic behavior and remains finite up to the surface, whereas the MTFA, as does the full theory, yields a decrease to zero. Quantitatively the agreement with the full theory is remarkable. Again for the highest donor concentration the deviation becomes larger. But this may be connected with the fact that in Ref. 1 another expression for $N_D^+(z)$ was used.

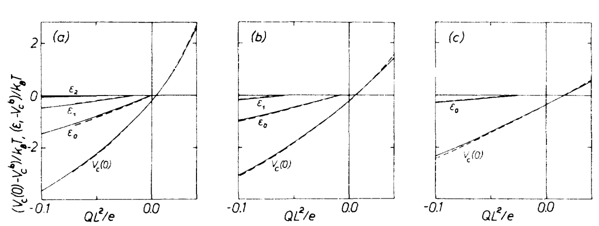

FIG. 1. For the three donor concentrations (a) $N_D^+=5\times10^{16}$ cm^{-3}, (b) 10^{17} cm^{-3}, and (c) 3×10^{17} cm^{-3} the subband energies E_i and the surface potential $V_c(0)$, both relative to the bulk potential V_c^b and in units k_BT, are shown vs the total carrier concentration Q per unit area (normalized as in Ref. 1: a unit length $L=4.62$ nm is used). The solid lines are the results obtained by the modified Thomas-Fermi approximation (MTFA) and the dashed lines are the results of Ehlers and Mills (Ref. 1).

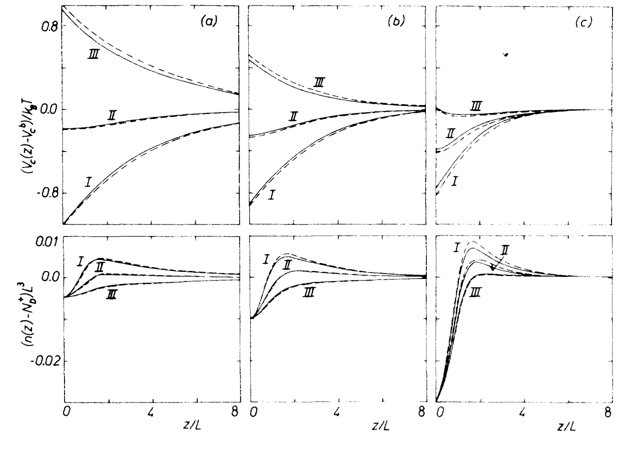

FIG. 2. For the three donor bulk concentrations given in Fig. 1 the upper row shows the spatial variation of the potential and the lower row the electron concentration for three values of Q: I $=-0.02e/L^2=-0.937\times10^{11}e/\mathrm{cm}^2$, II $=0.0e/L^2$, III $=0.02e/L^2$, respectively. The solid lines are the MTFA results and the dashed lines are calculated in Ref. 1.

In conclusion, the MTFA yields results for depletion and accumulation layers in good qualitative and quantitative agreement with a full self-consistent Hartree theory. This indicates that the deficiency of the conventional TFA is connected with the violation of the boundary condition for the wave functions at the surface, which is properly taken into account in the MTFA. At the same time the MTFA is numerically practically as simple as the usual TFA. In addition, contrary to the full self-consistent theory, the MTFA requires no different treatment for inversion, depletion, and accumulation. Finally, of course, the calculated potential can be fitted to analytic forms for further applications.

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