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# CALCULATIONS OF THE CRITICAL POINTS AND GROUND STATES FOR ELECTRON-HOLE DROPLET CONDENSATION IN SiC, GaP, AND AℓAs

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Theoretical results for the critical temperatures and densities and for the ground state energies and densities of electron-hole droplets in SiC, GaP, and AℓAs are reported. They are in good agreement with recent experimental results. Electron-phonon coupling and, in the cases of GaP and AℓAs, the camel's back conduction band structure are found to contribute significantly to the stability of the condensed state.

## I. Introduction

The most detailed experimental and theoretical studies of electron-hole droplet (EHD) condensation have been made in the elemental systems Ge and Si. Recently, however, experimental results for both the ground states and the critical points have become available for the compound systems GaP, SiC, and AℓAs [1].

These systems exhibit the highest values of the critical temperature $T_c$ observed experimentally to date. It has been suggested that two characteristics of these systems contribute to the stability of the EHD phase: (i) Electron-LO phonon coupling is believed to enhance the binding of the collective state relative to excitons [2]. The values of the Fröhlich coupling parameters for electrons are $\alpha \simeq 0.31$ for SiC, $\alpha \simeq 0.21$ for GaP, and $\alpha \simeq 0.26$ for AℓAs, and thus electron-phonon coupling is expected to be especially important in SiC. (ii) GaP and AℓAs are believed to exhibit the so-called camel's back structure at the bottom of the conduction band near the X point in the Brillouin zone because of the lack of inversion symmetry for the zincblende compounds [3]. The camel's back consists of two minima displaced somewhat from the X point along (100) in k space which lie a small energy $\Delta E$ below the X point value. This gives a large effective density of states near the bottom of the conduction band and thus lowers the cost in kinetic energy to form the collective state.

In the present note we give the results of the first detailed theoretical evaluations of the critical temperatures and densities for EHD condensation in these three systems. Detailed results for their ground state energies and densities are also given. The effects of electron-phonon coupling and of the camel's back conduction bands are taken into account. Inclusion of these features is found to be necessary to understand the high $T_c$, high ground state densities, and low ground state energies of these systems.

## II. Formalism and Ground State Calculations

The method used for treating the contributions to the energetics is now described, and results are given for the ground state energy $\varepsilon_o$ and density $n_o$. They are obtained from the minimum of the energy per electron-hole pair versus density in the dense electron-hole fluid

$$\varepsilon(n) = \varepsilon_k(n) + \varepsilon_{xc}(n), \tag{1}$$

where $\varepsilon_k$ is the contribution from the non-interacting kinetic energy, and $\varepsilon_{xc}$ is that from the exchange-correlation energy.

The coupled light and heavy hole valence bands and the conduction bands of SiC are parabolic and their contributions to $\varepsilon_k$ are obtained straightforwardly. The dispersion relations of the camel's back bands in GaP and AlAs, however, are more complex and give an effective density of states

$$D(E) \propto \{E + ((\Delta_o-\Delta)/2) + [((\Delta_o-\Delta)/2)^2 + \Delta_o E]^{\frac{1}{2}}\}^{\frac{1}{2}}, \tag{2}$$

for $E > 0$, and a corresponding expression for $E<0$. Here $\Delta$ is the splitting between the $X_1$ and $X_3$ conduction bands, and $\Delta_o$ is the corresponding splitting at the k value of the conduction band minimum. The parameters $\Delta$, $\Delta_o$, and $\Delta E$ for GaP are 355.5 meV, 427.1 meV, and 3.0 meV and for AlAs are 350.0 meV, 415.4 meV, and 2.57 meV. They were evaluated based on spectroscopic measurements and band structure calculations. The contribution to $\varepsilon_k(n)$ from the camel's back conduction bands is obtained by integrating Eq. (2) for each of the three bands.

Detailed calculations of $\varepsilon_{xc}(n)$ are not available for these systems. The combined $\varepsilon_{xc}(n)$ in effective atomic units, however, is nearly independent of band structure. We have used for $\varepsilon_{xc}(n)$ the detailed results [4] for six model systems based on Ge and Si. The present calculations have been performed using first the average of these values for the six model systems and secondly the values for Si[2;2]. The latter has band degeneracies similar to the present cases. As expected, our results are found to be fairly insensitive to the choice of $\varepsilon_{xc}(n)$; variations in $n_o$ corresponding to the two treatments are $\lesssim 4\%$. The results quoted here were obtained using $\varepsilon_{xc}(n)$ for Si [2;2].

| | SiC | GaP | AlAs |
|---|---|---|---|
| theory | | | |
| $\varepsilon_o$ (meV) | -42.5 | -30.2 | -45.9 |
| $n_o$ ($10^{18}$cm$^{-3}$) | 10.3 | 7.90 | 24.8 |
| experiment | | | |
| $\varepsilon_o$ (meV) | -44 ± 4 | -36.8 ± 3.0 | -42 ± 4 |
| $n_o$ ($10^{18}$cm$^{-1}$) | 10.0 ± 1.7 | 8.6 ± 1.5 | 16.0±1.0 |

Table I. Theoretical and experimental values of the ground state properties of electron-hole droplets: Experimental values are from Ref.[1]

The effects of electron-LO phonon interaction were included along the lines suggested by Keldysh and Silin [2] in which the leading order effect is to replace the bare carrier masses and

the high frequency dielectric constant with polaron masses and the low frequency dielectric constant. The next order contribution gives a further correction to the exchange energy.

The values of $\varepsilon_o$ and $n_o$ (Table I) calculated from Eq. (1) are seen to be in good overall agreement with experiment. The results for GaP are similar in essentials to those in Ref. [1]. The results for SiC use improved masses for the valence bands which include more fully the effects [5] of the coupling of the split-off spin-orbit band with the light hole valence band.

## III. Critical Point Calculations

The critical points were calculated using a method based on the uniform plasma approach introduced by Combescot [6]. In general, the critical point is given by an inflection point in the chemical potential $\mu$ versus n with temperature as a parameter. In the uniform plasma model $\mu$ is represented by that for a uniform dense electron-hole plasma; then if the critical point is found at high effective density, the approach is justified a posteriori.

It has been pointed out [7] that this approach provides a reliable upper bound for $T_c$ but that due to the neglect of statistical fluctuations, it overestimates somewhat the value of $T_c$. By making comparisons with experiment for Ge, Si, and for strained Si [8] and also with calculations which include fluctuations, it was found [7] that this approach gives a consistent overestimate of $T_c$ by $\simeq$ 20%. The uniform plasma approach has the merit of being relatively simple, and thus it can be generalized easily for complex systems such as the camel's back bands here.

The chemical potential is given by $\mu = \partial[nf(n,T)]/\partial n$ in terms of the free energy per pair f(n,T) and can be written

$$\mu = \mu_k(n,T) + \mu_{xc}(n) \quad . \tag{3}$$

Here $\mu_k$ is the contribution corresponding to non-interacting particles. $\mu_{xc}$ is the contribution from the Coulomb interactions, and it is taken to be independent of T because the exchange-correlation lowers the bands nearly rigidly.

| | SiC | GaP | AlAs |
|---|---|---|---|
| theory | | | |
| $T_c$ (°K) | 45 | 44 | 56 |
| $n_c$ ($10^{18}$cm$^{-3}$) | 2.2 | 0.53 | 1.72 |
| experiment | | | |
| $T_c$ (°K) | 41 | 45 | 52 |

Table II. Theoretical and experimental values for the critical points for EHD condensation: Experimental values are from Ref 1

For the parabolic bands we find that for all T up to $T_c$, $\mu_{ki}$, the contribution from band i, can be obtained by expanding to first order in $(k_BT/E_{Fi})$. For the camel's back conduction bands, however, no such expansion is possible because the density of states at low energy is large, and thus $E_{Fi}$ is small. For these cases $\mu_{ki}$ has been calculated exactly from the integral over the Fermi functior

$$n_i = \int_0^\infty D_i(E)\ [1+\exp(E-\mu_{ki})/k_BT]^{-1} dE\ . \qquad (4)$$

Results for the critical points are given in Table II. The values of $T_c$ were obtained by reducing those given by the uniform plasma approach by 20% to account for the effects of fluctuations. They are seen to be in reasonably good agreement with experiment. This tends to confirm that the simple uniform plasma approach when used in this way is useful for estimating the critical points of complex systems. Accurate experimental values of $n_c$ are not yet available.

## IV. Discussion

The present results for both the ground state properties and the critical points are in good overall agreement with experiments. This suggests that our understanding of the basic energetics of EHD in these compound systems is reasonably good.

These results have been checked by modifying the energetics in several ways. If the camel's back conduction bands of GaP and AℓAs are replaced by effective parabolic bands, agreement cannot be achieved with all of the experimental results. If the effects of the electron-LO phonon coupling are not included as above the $T_c$, $\varepsilon_o$, and $n_o$ are generally too small. Inclusion of the next order correction due to the electron-phonon coupling [5] leads to somewhat larger values of $\varepsilon_o$, $n_o$, and $T_c$ and to poorer overall agreement with experiment.

The present results can be used to check recently proposed scaling relations [9] between the ground state and critical parameters of EHD. These relations were developed for systems which have parabolic bands and no significant electron-phonon coupling. It is seen that the rule $\varepsilon_o/k_BT_c \simeq$ const and the rule relating $T_c$ and $n_o^{1/4}$ are satisfied reasonably well. On the other hand, the values of $n_c/n_o$ for the GaP and AℓAs are markedly less than the value $n_c/n_o \simeq .3$ proposed for systems with parabolic bands. This difference arises because the energy (density) dependence of the density of states for electrons in systems with camel's back bands is different in the region of $n_o$ and the region of $n_c$.

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