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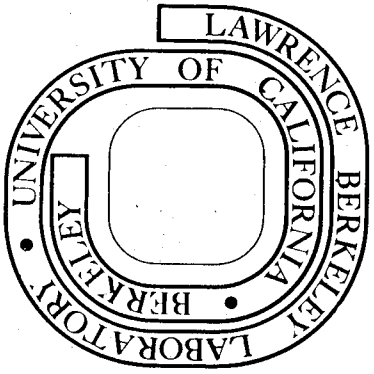

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DENSITY VARIATION IN THE STRAIN-CONFINED ELECTRON-HOLE LIQUID IN Ge*

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In this paper we theoretically analyze two mechanisms which could account for the experimentally observed increase in pair density for the strain confined electron-hole liquid (EHL) in Ge. We find that the change in drop density with uniform stress is insufficient to explain the experimental result. However, we find that the strain gradient in the well acts to compress the liquid sufficiently to explain the observed density increases. Densities of twice the equilibrium value can be easily obtained for large enough drop size, but the density should vary by < 10% if the drop radius is < 100 μm.

LARGE, LONG-LIVED electron-hole drops (EHD) can be produced in a potential well induced in an inhomogeneously-strained Ge crystal.[1,2,3] If such a drop (γ-drop) is small enough, the electron-hole pair density n inside the liquid is essentially uniform. Experimentally, this can be determined by measuring either the luminescence lineshape or the recombination lifetime as a function of drop size (varied by changing the laser pump power P). For small enough γ-drops, the luminescence linewidth ΔE (proportional to the Fermi energy) and recombination lifetime τ_o (approximately proportional to n^{-1}) both have constant values independent of drop size. However, for drops with radius larger than $R \approx 150\ \mu$, both ΔE and τ_o^{-1} begin to increase with drop size, indicating that the average density in the liquid is increasing.

There are at least two mechanisms which could be responsible for an increase in n. First, n should change with uniform stress. It has been shown theoretically[4,5,6] that, for uniaxial stress along a $\langle 111 \rangle$-crystal axis,[7] the equilibrium density should decrease by a factor of 20 in going from zero stress to a high stress limit. As the γ-drop grows in the strain well, liquid is pushed into regions of lower strain, where the equilibrium density may be higher. A second mechanism for raising the density is an actual compression of the liquid in the well: as the drop grows with P, liquid is forced into regions of higher energy, and the drop can lower its total energy by increasing the pair density in the low energy regions near the center of the drop. The purpose of this paper is to quantitatively compare these two mechanisms for increasing the drop density. We find that most of the density increase is due to compression, and that over the experimental range of stresses, the density does not change greatly with uniform stress.

We write the energy per pair in the liquid as the usual sum of kinetic, exchange, and correlation energy contributions:

$$E = E_K + E_X + E_C \qquad (1)$$

The exchange energy includes the corrections for carrier mass anisotropy and valence band degeneracy[8] as calculated by Combescot and Nozières.[5] The form for the correlation energy is discussed below. Our calculations assume that only one conduction band minimum is

occupied, and hence are valid only for compressional stresses greater than about 3 kg/mm^2. (Only for ⟨ 111 ⟩-stresses larger than this is the drop attracted to regions of higher strain.[3])

At each stress the energy, Eq. (1), is minimized with respect to density, and the resulting equilibrium values n_o and E_o are plotted in Figs. (1) and (2). In each figure the three curves correspond to three models of the correlation energy, E_C. In the first two models, both the exchange and the correlation energy are taken to be independent of stress. The entire stress dependence comes from changes in hole kinetic energy as the two valence bands are split by stress. The hole kinetic energy [$E_K^h(n)$] at T = 0 is found by numerical integration over the full strain-split hole bands.[9] Model 1 employs a detailed numerical calculation[10] for the correlation energy valid in the low stress limit [Ge (1:2) in the notation of Ref. 3]. The results of this calculation were kindly supplied to us by Dr. Vashishta. In model 2, this detailed calculation is replaced by a simple empirical correlation energy, given as the sum of Wigner-type contributions from the electrons and holes[11]

$$E_C = -\frac{C}{n^{-1/3}+A/m_{oe}} - \frac{C}{n^{-1/3}+A/m_{oh}} \qquad (2)$$

Here $m_{oe} = 3(m_\ell^{-1} + 2m_t^{-1})^{-1} = 0.12\ m_o$ is the electron optical mass,[4] and m_{oh} is an approximate hole optical mass given by

$$2m_{oh}^{-1} = m_{HH}^{-1} + m_{LH}^{-1} \qquad (3)$$

where m_{HH} and m_{LH} are heavy and light hole masses, and $m_{oh} = 0.075\ m_o$. This mass is the correct optical mass to use in the high stress limit, and has been used as well[4,6] in calculating the binding energy in unstressed Ge. A and C are parameters whose values are adjusted to yield Vashishta's[10] equilibrium values of E_o and n_o in the zero-stress limit. It can be seen that these two models give results in reasonable agreement, and also agree approximately in the high-stress limit with the calculations of Ref. 6. In model 3 we attempt to estimate the importance of the change in correlation energy with stress: E_C is given by an expression of the form of Eq. (2), but now m_{oh} is given by[12]

$$m_{oh}^{-1} = \frac{N_{HH}}{N} m_{oHH}^{-1} + \frac{N_{LH}}{N} m_{oLH}^{-1} \qquad (4)$$

where N_{HH}/N is the fraction of holes in the heavy hole band, $N_{HH} + N_{LH} = N$, and C and A are recalculated. The optical masses m_{oHH} and m_{oLH} are calculated numerically by integrating over the Fermi surface:

$$\frac{N_{HH}}{m_{oHHij}} = + \frac{1}{4\pi^3\hbar^2}\int \frac{\partial E}{\partial k_i}\frac{\partial E}{\partial k_j}\delta(E-E_F)d^3k \qquad (5)$$

For a ⟨ 111 ⟩-stress, m_{oHHij} is diagonal with longitudinal and transverse components, and $3m_{oHH}^{-1} = m_{oHH\ell}^{-1} + 2m_{oHHt}^{-1}$. The resulting hole optical mass varies from 0.25 m_o to 0.075 m_o[13] as the stress varies from 0 to $-\infty$. (Compressional stresses are taken to be negative.) The resulting n_o and E_o derived from this model differ discernibly from the results of the other models, especially in the region of experimental interest ($-\sigma$ = 3-10 kg/mm^2), and it would be of interest to attempt a more detailed calculation of E_C at finite stress.

In all three models, however, most of the change in density occurs after one hole band is completely depopulated, as indicated by the arrows in Fig. 1. For lower stresses, the change in n is too small to explain the observed[14] power dependence of the γ-drop linewidth or lifetime. For example, for typical experimental conditions the equilibrium pair density could not vary by more than 35% over the entire well ($-\sigma$ = 3-6 kg/mm^2), unless compressional effects are considered. Experimentally, the density is observed to increase by ≈ a factor of two for drops of radius 400 μm.[15]

The compression of the strain-confined liquid may easily be estimated. Inside the γ-drop the carriers adjust the local density so that the chemical potential is constant throughout the drop volume. At T = 0, the chemical potential can be written

$$\mu = E + \frac{p}{n} + E_s \qquad (6)$$

where E is the energy per pair, p is the fluid pressure, n is the density, and E_s is the strain energy. E is given by Eq. (1), which for small deviations from the equilibrium density may be approximated

$$E = E_o + \frac{1}{2} E''_o (n-n_o)^2 \ , \qquad (7)$$

where E_o and n_o are the equilibrium pair energy and density, and E''_o is related to the compressibility. The pressure is then given by

$$p = n^2 \frac{\partial E}{\partial n} = n^2 E''_o (n-n_o) \ . \qquad (8)$$

Near the bottom of the potential well, the strain energy is approximately parabolic:

$$E_s = \alpha r^2 \qquad (9)$$

where $\alpha \simeq 8$ meV/mm^2 for a stress of ~ -5.5 kg/mm^2 along a $\langle 111 \rangle$ crystal direction.[3]

Keeping only terms linear in $(n-n_o)$, Eq. (6) may be written

$$\mu = E_o + n_o E''_o (n-n_o) + \alpha r^2 = \text{const.} \qquad (10)$$

The constant is determined by the boundary condition that p be continuous across the surface.[16] At low T the gas pressure outside the drop can be neglected, so that

$$n(r=R) = n_o \qquad (11)$$

where R is the drop radius. In this case, Eq. (10) yields

$$n(r) = n_o [1 + \hat{\alpha} (R^2 - r^2)] \qquad (12)$$

where $\hat{\alpha} = \alpha/(n_o^2 E''_o)$. Vashishta[10] has calculated $n_o^2 E''_o = .62$ meV for Ge(1:2). This compression is large enough to explain the experimental effects. For example, for a 400 μm radius drop, Eq. (12) predicts $n(r=0) \approx 3\, n_o$. However, if the drop has a radius less than 100 μm, the density will be within 10% of the equilibrium value throughout the drop.

It is interesting to note that the compression predicts that the density should be higher in the center of the drop, while a variation in density with uniform stress predicts that the density should be higher at the surface of the drop.[17] It has in fact been found[15] that the density is higher at the center of the drop, thus confirming the theoretical ideas presented here. In a later publication,[18] a more complete theoretical and experimental determination of n(r) will be presented.

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* Supported in part by the U.S. Energy Research and Development Administration.

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8. The exchange energy of the holes should vary by ~ 25% with stress. This effect is ignored here and the low stress exchange energy is used.
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16. The change in pressure crossing the drop surface is proportional to the surface tension, but this correction generally has a negligible effect.
17. In model 3, there is a range of stress for which n would be highest at the drop center. However, the average density would then decrease as the drop size increased, contrary to the experimental results of Refs. 14 and 15.
18. KELSO S.M., *et al.*, to be published.

FIGURE CAPTIONS

Figure 1. Theoretical equilibrium pair density n_o inside an EHD, plotted as a function of ⟨ 111 ⟩ uniaxial stress. The three different curves (labelled 1, 2, 3) represent three approximations to the correlation energy, as discussed in the text. The calculations assume only one conduction band ellipsoid is occupied, and hence can be compared to experiment only for $|\sigma| \gtrsim 3$ kg/mm^2. The dashed line at $n_o = 1.1 \times 10^{16}$ cm^{-3} is Vashishta's more accurate theoretical result (Ref. 6) for the high-stress limit. All three curves are constrained to agree with Vashishta's zero-stress result (Ref. 10). The arrows indicate the stress at which one hole hand is just depopulated (at T = 0 K). Note the scale change at $-\sigma = 10$ kg/mm^2.

Figure 2. Theoretical binding energy E_o per pair in an EHD, with respect to the unfilled conduction band, plotted as a function of ⟨ 111 ⟩ uniaxial stress. The three solid curves are as in Figure 1. The dashed line at -3.08 meV is Vashishta's result (Ref. 6) for the high-stress limit.

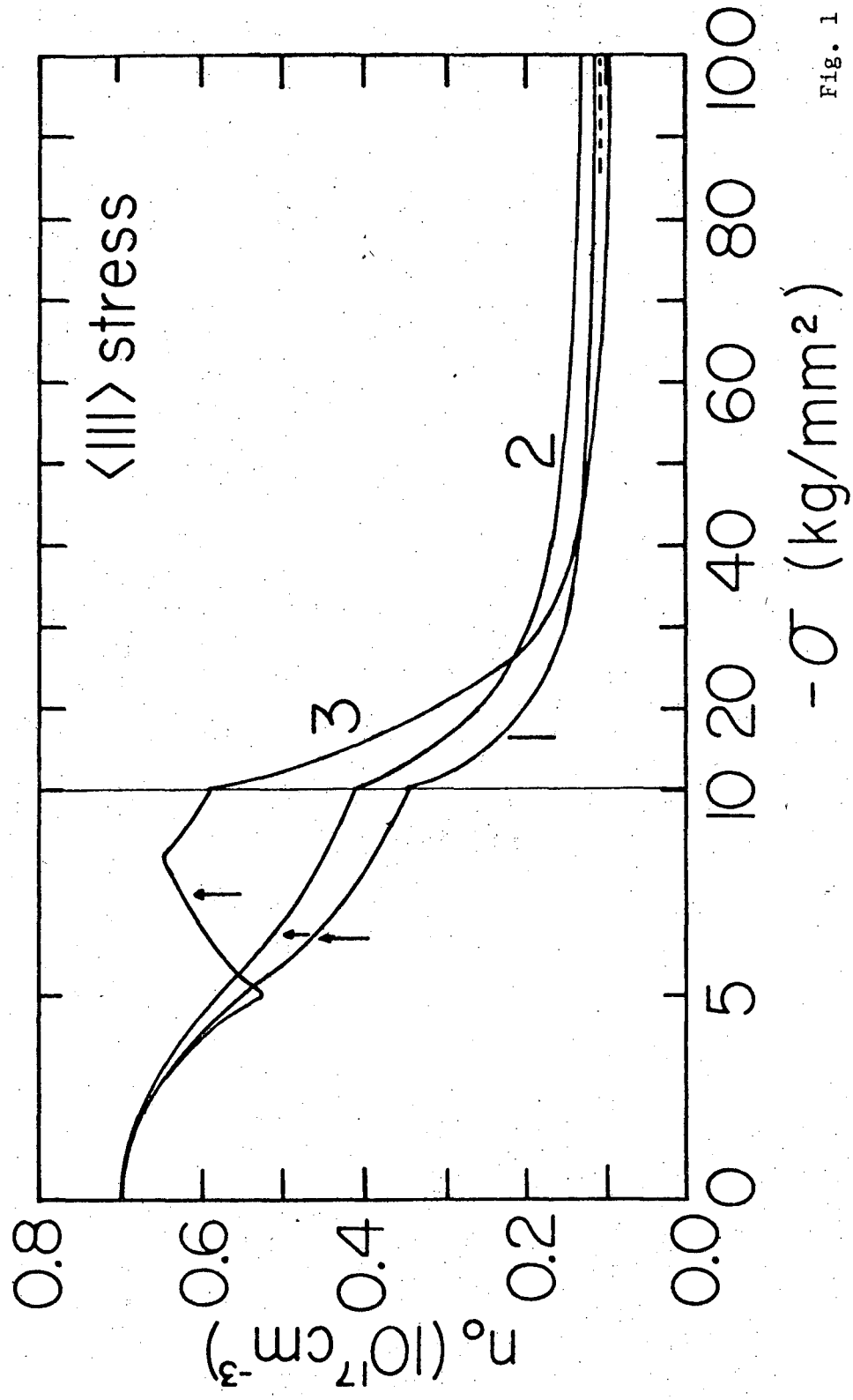

Fig. 1

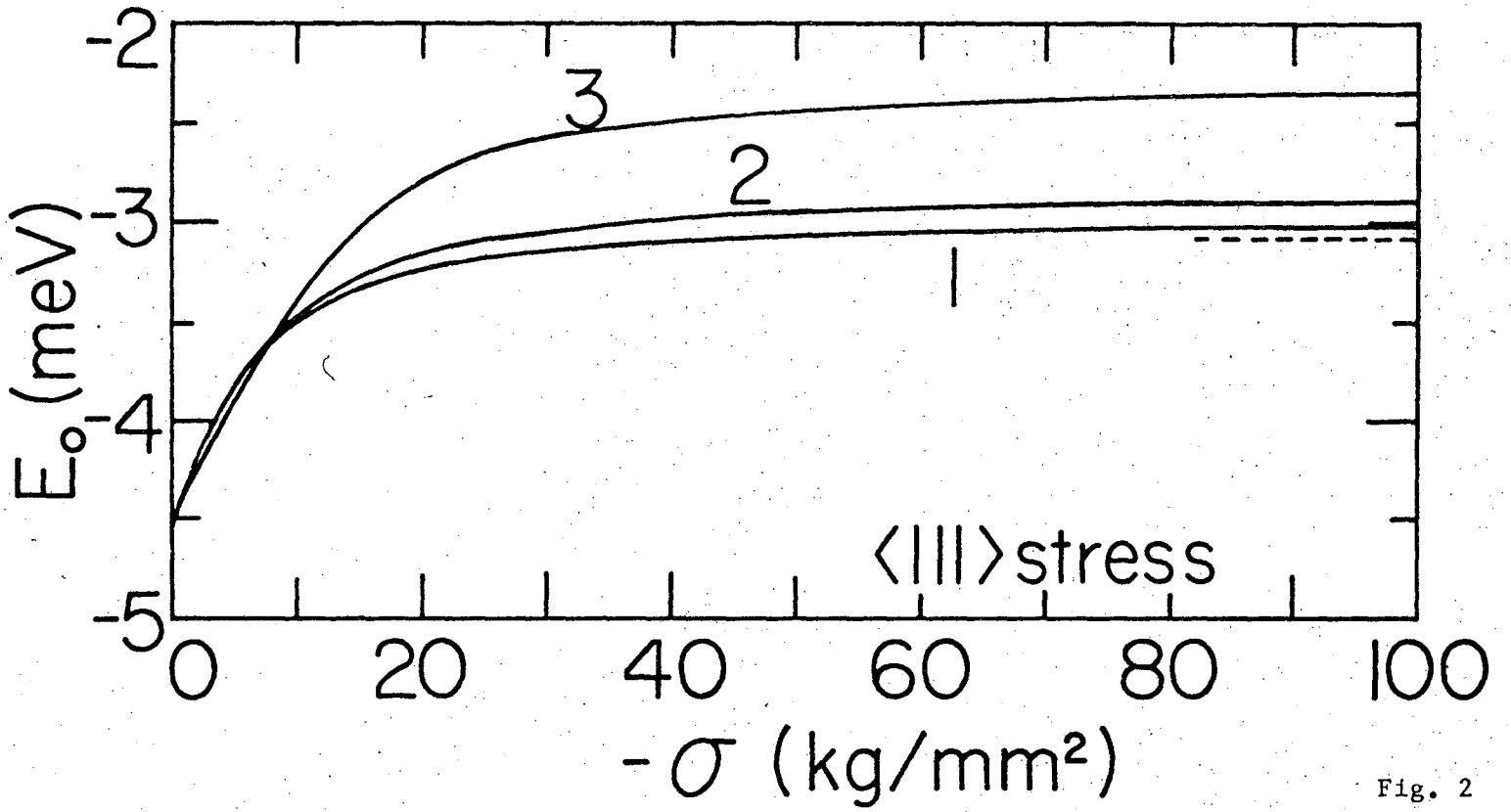

Fig. 2

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