ON THE SHAPE OF THE DROPLET IN UNIAXIALLY STRESSED Ge

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ABSTRACT

Density functional formalism developed by Hoenberg, Kohn, and Sham is applied to the calculation of the surface tension of electron-hole droplets in uniaxially stressed Ge. It is shown that the shape of droplets in highly excited Ge under a uniaxial stress of about 0.3 k bar along the [111] direction is oblate spheroid because of the anisotropy of electron mass parameter. The ratio of the minor axis to the major one is estimated to be at most 1.9.

Determination of the shape of droplet by the light scattering experiment is discussed.

I. INTRODUCTION

Combescot and Nozieres,[1] Brinkman and Rice,[2] and Vashishta *et al.*[3] have estimated the binding energy per electron-hole pair in droplets of stressed Ge and Si by using the theory of uniform electron-hole liquid; in which the surface energy was not considered explicitly. Theoretical investigation on the surface property of droplets has been done so far for unstressed Ge.

The minima in the conduction band of Ge consist of four ellipsoidal valleys. Although each valley is anisotropic, the symmetry of the whole valleys is cubic. Therefore the mass anisotropy of each valley does not influence on the surface property of droplets such as surface tension in unstressed Ge.

Benoit à la Guillaume and Voos[6] observed electron-hole drops in uniaxially stressed Ge. In their experiment Ge is uniaxially stressed with the pressure of about 0.3 k bar in the [111] direction, so that conduction electrons in the droplets belong only to [111] valley, while holes in the droplets still consist of the heavy and light ones.

The aim of this report is to make clear theoretically the effect of the mass anisotropy on the surface tension of droplets in properly stressed Ge.

In what follows we employ units of $\hbar=m_0=1$ (where m_0 is electron mass in vacuum) but electron charge e is conserved.

II. DENSITY FUNCTIONAL FORMALISM AND SCALE TRANSFORMATION

Let us consider a droplet consisting of fixed number N of electron hole pairs in stressed Ge.

According to Benoit à la Guillaume and Voos's experiment[6] we deal with only one electron valley with anisotropic masses ($m_{e\parallel}$, $m_{e\perp}$) and one isotropic hole band for simplicity. We use the number density functional formalism developed by Hoenberg, Kohn and Sham.[7,10] The ground state energy of the droplet is given as a functional of the electron density $n^e(\vec{r})$ and hole density $n^h(\vec{r})$ by

$$
\begin{aligned}
&E_{NG}(n^e(\vec{r}),\ n^h(\vec{r})) \\
&= \int d\vec{r}\ \Big[\ \varepsilon_{NG}(n^e(\vec{r}),\ n^h(\vec{r})) \\
&\quad + A_{\parallel}(n^e,\ n^h)(\vec{\nabla}_{\parallel} n^e)^2 + A_{\perp}(n^e,\ n^h)(\vec{\nabla}_{\perp} n^e)^2 \\
&\quad + B_{\parallel}(n^e,\ n^h)(\vec{\nabla}_{\parallel} n^h)^2 + B_{\perp}(n^e,\ n^h)(\vec{\nabla}_{\perp} n^h)^2 \\
&\quad + C_{\parallel}(n^e,\ n^h)(\vec{\nabla}_{\parallel} n^e)(\vec{\nabla}_{\parallel} n^h) + C_{\perp}(n^e,\ n^h)(\vec{\nabla}_{\perp} n^e)\cdot(\vec{\nabla}_{\perp} n^h) \\
&\quad + O(\nabla^4) + \cdots \qquad \Big] \\
&\quad + \frac{e^2}{2\epsilon_0}\iint d\vec{r}d\vec{r}'[(n^h(\vec{r}) - n^e(\vec{r}))(n^h(\vec{r}') - n^e(\vec{r}'))/|\vec{r} - \vec{r}'|\ ]. \qquad (2.1)
\end{aligned}
$$

The gradient dependent terms come from variation of the carrier densities and the coefficients $A_{\parallel}$, $A_{\perp}$, $B_{\parallel}$, $B_{\perp}$, $C_{\parallel}$ and $C_{\perp}$ are connected with the proper polarization parts of uniform electron-hole liquid.[7] Hereafter we take into account up to second order in the gradient expansion. The notations $\parallel$ and $\perp$ mean the directions parallel and perpendicular to [111] respectively.

We make use of R.P.A. in calculation of these coefficients $A_{/\!/}$, $A_{\perp}$, $B_{/\!/}$, and so forth and furthermore assume local neutrality;

$$n(\vec{r}) \equiv n^e(\vec{r}) = n^h(\vec{r}) . \tag{2.2}$$

Then after some mathematical manipulations

$$E_{NG} = \int d\vec{r}\{ \varepsilon_{NG}(n,n) + \frac{1}{72n} [(\frac{1}{m_{e/\!/}} + \frac{1}{m_h})(\vec{\nabla}_{/\!/} n)^2 + (\frac{1}{m_{e\perp}} + \frac{1}{m_h})(\vec{\nabla}_{\perp} n)^2] \} \cdots , \tag{2.3}$$

where $m_{e/\!/}(=1.58)$ and $m_{e\perp}(=0.082)$ are the masses of electron parallel and perpendicular to the [111] direction, respectively and m_h is the hole mass. It should be noted that the gradient terms in eq.(2.3) come from kinetic energies and do not depend upon electron charge e.

The coefficients of the second term in eq.(2.3) is smaller than that of the third term. The second term determines the surface energy $S_{/\!/}$ of the surface whose normal vector is parallel to the [111] direc tion and the third term determines the surface energy $S_{\perp}$ of the surface whose normal vector is perpendicular to the [111] direction.

Because $S_{/\!/}$ is smaller than $S_{\perp}(S_{/\!/} < S_{\perp})$ we can expect that the stable shape of the droplet is not spherical but oblate-spheroidal. In order to determine the shape quantitatively, we perform scale transformation of coordinate. The new coordinate $\tilde{\vec{r}}$ is defined by

$$\tilde{\vec{r}}_{/\!/} \equiv (\frac{M_{/\!/}}{M_{\perp}})^{1/3} \vec{r}_{/\!/} , \qquad \tilde{\vec{r}}_{\perp} \equiv (\frac{M_{\perp}}{M_{/\!/}})^{1/6} \vec{r}_{\perp} , \tag{2.4}$$

where

$$\frac{1}{M_{/\!/}} = \frac{1}{m_{e/\!/}} + \frac{1}{m_h} , \qquad \frac{1}{M_{\perp}} = \frac{1}{m_{e\perp}} + \frac{1}{m_h} . \tag{2.5}$$

The density in the scaled coordinate $\tilde{n}(\tilde{\vec{r}})$ should be defined to equal to $n(\vec{r})$ since the volume element is conserved in transformation to the new coordinate.

The gradient terms appearing in energy functional become spherical in this scaled coordinate $\tilde{\vec{r}}$ as

$$E_{NG} = \int d\vec{\tilde{r}} \, [\varepsilon_{NG} + \frac{1}{72M^{2/3}M^{1/3}\tilde{n}(\vec{\tilde{r}})} \, | \vec{\tilde{\nabla}}\tilde{n}(\vec{\tilde{r}}) \, |^2 \,]. \qquad (2.6)$$

If the density distribution $\tilde{n}_G(\vec{\tilde{r}})$ minimizing the density functional E_{NG} is unique, this distribution should be a spherical function of $\vec{\tilde{r}}$ from symmetrical consideration. This means that the shape of the droplet is oblate-spheroidal in the ordinary coordinate.

The ratio of the minor axis parallel to [111], $R_{/\!/}$, to the major one perpendicular to [111], $R_{\perp}$ is given by

$$\frac{R_{\perp}}{R_{/\!/}} = \left(\frac{\frac{1}{m_{e_{\perp}}} + \frac{1}{m_h}}{\frac{1}{m_{e_{/\!/}}} + \frac{1}{m_h}} \right)^{1/2} \qquad (2.7)$$

from the definition of the scaled coordinate $\vec{\tilde{r}}$. The mass m_h is determined as the average value of those of heavy and light ones, m_{hh} and m_{lh};[11)]

$$\frac{1}{m_h} = \frac{\alpha_{hh}}{m_{hh}} + \frac{\alpha_{lh}}{m_{lh}} \; , \qquad \alpha_{hh} + \alpha_{lh} = 1, \qquad (2.8)$$

where α_{hh} and α_{lh} are the rates of the densities of heavy hole and light hole. Assuming that the hole bands are degenerate at Γ point and using the values m_{hh}=0.347, m_{lh}=0.042 we get m_h=m_{hh}/1.3 and from (2.7) the value of $R_{\perp}/R_{/\!/}$ is 1.9.

III. EFFECT OF EXCHANGE ENERGY AND CORRELATION ENERGY

When we go beyond R.P.A., taking into account the contribution to the properpolarization parts of electron-hole liquid from exchange and correlation energy roughly,[9,10)] we may estimate the ratio of the axes to be larger than 1.2.[11)] After all we may expect the ratio of the axes is between 1.2 and 1.9.

IV. LIGHT SCATTERING EXPERIMENT

The warping of the droplet discussed so far can be measured in a

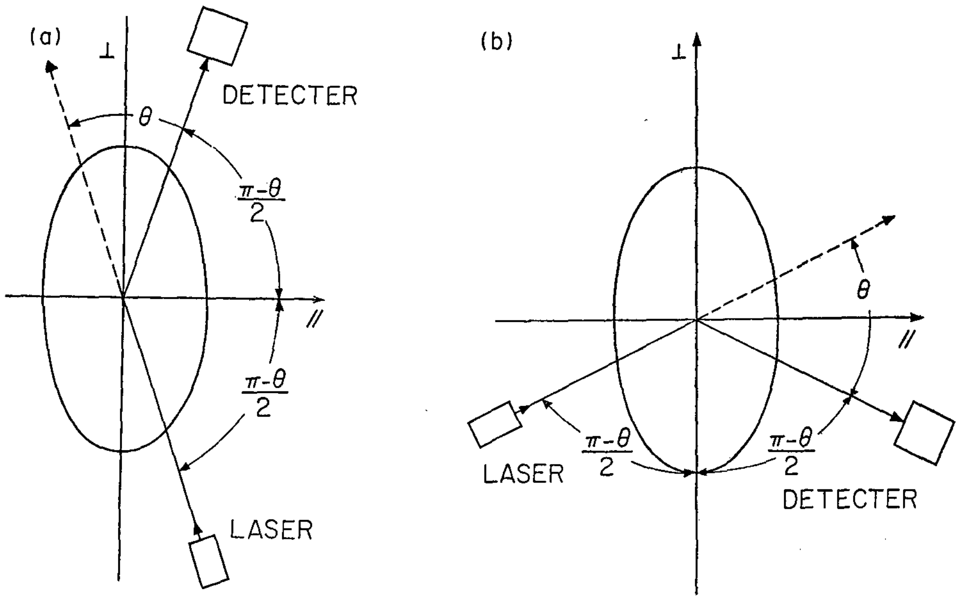

Fig.1. The symbols // and ⊥ denote the direction parallel and perpendicular to the [111] direction. A droplet is represented as an ellipsoid.

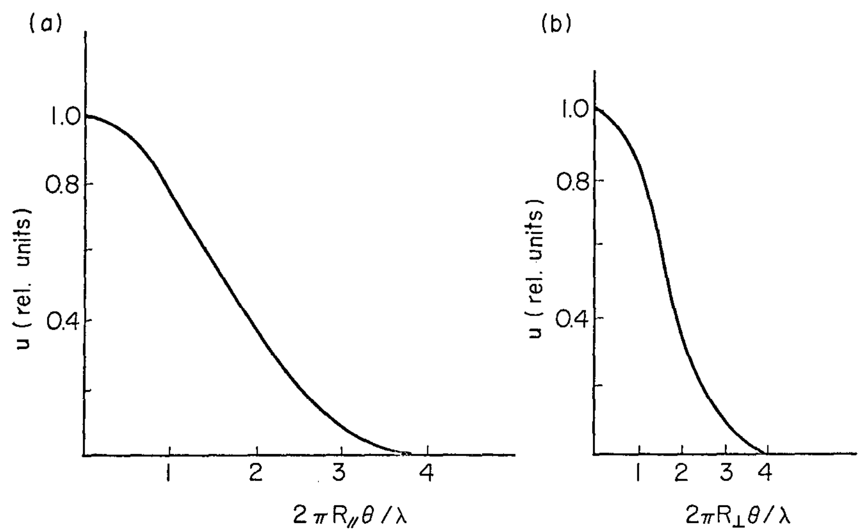

Fig.2. The angle distribution of the scattered light.
Fig.2a corresponds to Fig.1a and Fig.2b to Fig.1b.
The unit of the abscissa in Fig.2a is $\lambda/2\pi R_{//}$ and that in Fig.2b $\lambda/2\pi R_{\perp}$,
Note that $1/R_{//}$ is larger than $1/R_{\perp}$.

light scattering experiment. The interesting geometries in the case of deformed droplet are sketched in Fig.1a and Fig.1b. A droplet is represented as an ellipsoid. The He-Ne laser and the detector of scattered light should be moved relatively to the sample crystal so as to keep the bisect between the incident beam and scattered light in the [111] direction or the direction perpendicular to [111], respectively.[11]

The angular distribution of the scattered light for the cases (a) and (b) are shown in Fig.2a and Fig.2b. We can observe that the axis ratio $R_{\perp}/R_{/\!/}$ is given by the ratio of half widths in Fig.2a and Fig.2b.

V. CONCLUSION

In conclusion, the shape of the droplet in properly stressed Ge is oblate spheroid and the ratio of minor axis to major one is at most 1.9.

REFERENCES

1) M. Combescot and P. Nozieres: J. Phys. C5 (1972) 2369.

2) W. Brinkman and T. M. Rice: Phys. Rev. B7 (1973) 1568.

3) P. Vashishta, P. Bhattacharyya, V. Massida, K. S. Singwi and P. Vashishta: Phys. Rev. B10 (1974) 5127.

4) T. M. Rice: Phys. Rev. B9 (1974) 1540.

5) L. M. Sander, H. B. Shore and L. J. Sham: Phys. Rev. Letters 31 (1973) 533.

6) C. Benoit à la Guillaume and M. Voos: Phys. Rev. B5 (1972) 3079.

7) P. Hoenberg and L. J. Sham: Phys. Rev. 136 (1965) B864.

8) W. Kohn and L. J. Sham: Phys. Rev. 140 (1965) A133.

9) L. J. Sham: *Computational Methods in Band Theory* ed. by P. M. Marais, J. F. Jank and A. R. Williams (Plenum, New York, 1971) p.458.

10) S. K. Ma and K. A. Bruckner: Phys. Rev. 165 (1968) 18.

11) M. Morimoto, K. Shindo and A. Morita: J. Phys. Soc. Japan 41 (1976) 91.

12) Y. Pokrovskii: ZhETF Pis. Red. 9 (1969) 435 [Soviet Physics -

JETP Letters 9 (1969) 261.]

13) H. C. Van de Hulst: *Light Scattering by Small Particles* (Wiley, N.Y., 1957) p.93.

14) L. D. Landau and E. M. Lifshitz: *Statistical Physics* (Pergamon, N.Y., 1958) p.458.