

# Effect of crystal lattice on the equilibrium shape of electron-hole drops

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The formation of electron-hole drops leads to an equilibrium deformation of the crystal lattice. It is shown that as a result of the anisotropy of the elastic properties of the crystal, drops of sufficiently large volume should be disk-shaped.

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The influence of external deformation on the behavior of electron hole drops (EHD) was investigated in a number of studies (see, e.g.,<sup>[1,2]</sup>). It will be shown below that the very appearance of the drop is accompanied by an equilibrium deformation of the crystal, so that the region of the crystal inside the drop turns out to be elongated (in the case of silicon and germanium), and slightly compressed outside the drop. The deformation, being small, does not affect the volume properties of the EHD; in a number of phenomena governed by surface tension, however, equilibrium deformation can exert a substantial action on the drop.

To estimate the characteristic values of the deformation and of the pressure, we consider a spherical drop placed in an isotropic elastic medium. The energy density of a crystal eith and EHD, with allowance for the electron-phonon interaction, can be written in the form

$$E = E_{el} + \frac{1}{2} \lambda u^2(\mathbf{r}) - Dn(\mathbf{r}) u(\mathbf{r}), \quad (1)$$

where  $E_{el}$  is the electron-hole contribution to the energy (with allowance for the surface energy),  $\lambda = (c_{11} + 2c_{12})/3$ ,  $c_{11}$  and  $c_{12}$  are the elastic moduli,  $u(\mathbf{r})$  is the strain,  $D$  is the summary deformation potential of the electrons and holes,  $n(\mathbf{r})$  is the coordinate-dependent density of the electrons and holes ( $n(\mathbf{r}) = n_0$  at  $|\mathbf{r}| < R$ ,  $n(\mathbf{r}) = 0$  at  $|\mathbf{r}| > R$ ,  $R$  is the radius of the drop).

The electron-phonon interaction produces elastic stresses  $\sigma(\mathbf{r}) = \partial E / \partial u(\mathbf{r})$  that lead to deformation of the medium. The determination of the equilibrium deformation is analogous to the problem of the thermoelastic stresses produced in a medium by a uniformly heated sphere.<sup>[3]</sup> The crystal region inside the drop turns out to be uniformly stretched (the width of the forbidden band inside the gap is smaller than on the outside) and the value of the strain is  $u_0 = Dn_0/\lambda$ ; outside the drop, the relative change of the volume is equal to zero, but the radial and tangential components of the stress do exist and decrease in proportion to  $1/r^3$ . There is therefore a strain gradient near the surface and gives rise to pressure on the drop. The force acting on a surface-layer element of the drop, with area  $S$  and thickness  $d$ , is equal to  $F = DnSd \text{ grad } u$ . Putting  $\text{grad } u \approx u_0/d$ , we obtain

$$p = \frac{F}{S} = \frac{(Dn)^2}{\lambda} \quad (2)$$

For germanium, substituting in (2) the values  $D \approx 3$  eV,  $\lambda = 10^{12}$  dyn/cm<sup>2</sup>, and  $n = 2 \times 10^{17}$  cm<sup>-3</sup>, [4] we find that the additional pressure on the drop surface is  $p_0 \approx 1$  dyn/cm<sup>2</sup>, and the relative crystal deformation is  $u_0 \approx 10^{-6}$ .

Let us compare  $p_0$  with the pressure due to the surface tension  $p' = 2\alpha/R_0$ . Putting  $\alpha = 2 \times 10^{-4}$  erg/cm<sup>2</sup> we obtain that  $p' < p_0$  at a drop radius  $R_0 > 4$   $\mu$ m.

The onset of deformation lowers the total energy of the drop; it follows from [1] that for a drop of radius  $R \approx 4$   $\mu$ m the energy decrease  $\Delta E$  amounts to  $\sim 1$  eV.

The elastic deformation of the medium in which the drops are located can lead to a number of effects. Thus, for example, a) elastic forces that decrease like  $1/r^3$  should act between the drops, in analogy with the forces acting between the dilatation centers in a cubic crystal<sup>[5]</sup>; b) in a cubic crystal the anisotropy of the elastic properties should lead (for drops of sufficiently large volume) to a stronger shape anisotropy. We shall dwell on this question in somewhat greater detail.

The equilibrium shape of the drop in the crystal is determined by the minimum of the total energy. In an anisotropic crystal, both the energy of the surface tension and the exchange energy of the elastic deformation of the lattice depend on the shape of the drop. The anisotropy of the elastic moduli causes the minimum of the elastic energy to correspond to an equilibrium drop shape in the form of a thin disk oriented along the easy compression axis (the [100] axis in Ge and Si). A similar "leveling" of other inclusions in cubic crystals is described in detail in<sup>[6]</sup>. The transformation of a small-volume drop into a disk is hindered by the increase of its surface energy. The critical volume at which the drop assumes abruptly the shape of a disk can be determined by considering the change of the energy at small deviations of the shape of the drop from spherical (i.e., by expanding the energy in capillary oscillations). The most unstable are ellipsoidal deviations from spherical form ( $n=2$ ).

The frequency of such oscillations vanishes at  $R_c \approx 3$   $\mu$ m. It turns out that in this case a jump into a disk-shape state takes place, with  $\delta = d/l \approx 0.5$  ( $d$  is the drop thickness and  $l$  is its diameter).

The cubic deformation of the drop, which occurs at any volume and is proportional to its mean radius, corresponds to capillary oscillations with  $n \geq 4$ . It turns out to be relatively small (at  $R \leq R_c$ ) because of the high frequency of these oscillations.

When the total volume of the drop is large enough, and consequently the drop is disk-shaped, its elastic energy is equal, in the zeroth approximation in  $d/l$ , to the energy of an infinitesimally thin plate.

For a disk of finite thickness, the elastic energy can therefore be represented in the form of the energy of an infinitesimally thin plate and an edge contribution proportional to  $d/l$ .

With decreasing  $d/l$ , the edge elastic energy decreases and the surface

energy increases; the equilibrium shape of a drop of volume  $V$  is consequently determined by the balance of the surface energy and the elastic edge energy:

$$\frac{(Dn)^2}{c_{11} + 2c_{12}} V \frac{d}{l} \approx l^2 \alpha. \quad (3)$$

Equation (3) takes into account the fact that the anisotropy of the elastic moduli is large, so that the anisotropic part of the elastic energy is of the same order as the elastic energy itself.

It follows from (3) that

$$d/l \approx (r_0/R)^{3/2}, \quad \text{where } r_0 = \alpha/\lambda u_0^2.$$

For example, a drop of radius  $10 \mu\text{m}$  should turn into a disk with a ratio  $d/l \approx 1/4$ .

We note in conclusion that no spontaneous uniaxial deformation can set in as a result of the splitting of the electron (hole) states, since a small splitting does not lower the total energy of the drop.

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<sup>2</sup>Ya. E. Pokrovskii, *Phys. Status Solidi A* **11**, 385 (1972).

<sup>3</sup>L. D. Landau and E. M. Lifshitz, *Teoriya uprugosti* (Theory of Elasticity), M. 1974. [Pergamon 1976].

<sup>4</sup>P. G. Baranskii *et al.*, *Poluprovodnikovaya élektronika* (Semiconductor Electronics), M. 1974.

<sup>5</sup>J. D. Eshelby, *Solid State Physics*, Vol. 3, New York, 1956, p. 79.

<sup>6</sup>A. G. Khachaturyan, *Teoriya fazovykh prevrashchenii i struktura tverdykh rastvorov* (Theory of Phase Transitions and Structure of Solid Solutions), Nauka, 1974.