On size of quantum bag and cracking

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Abstract

This paper deals with the size limit of material micro and nano-structure associated with its energy state of stability. From the viewpoint of mechanics, there exists the competition between the surface tension and coulomb factor in the electron layer on the surface of bulk. When the bulk size reduces to nm size, the surface effect is comparable to the bulk. The system could collapse into new many-body quantum state. Based on the revised Thomson-Fermi-Dirac(TFDC) theory, the limiting size of a stable material nano structure is obtained. The value of limiting size is of the order "nm" by a crude estimation for water.

1. Introduction

A modified Thompson-Fermi-Dirac (TFD) model [1] consists of a shell of electron cloud of tunneling electrons. It encloses the bulk material and shall be referred to as the "Quantum Bag". The shell of electrons prevails by two factors. One is the surface tension γ that exerts an inward pressure to the bulk material. The other gives an outward extension due to a double charge layer with opposite sign. For a large bulk, the surface tension is less effective than the coulomb factor. As the bulk decreases in size, the surface effect begins to dominate. Then, the crust of the shell will break and cracks would start. Hence, there exists a limit size for the bulk to be stable RL, below which the shell would not be tenable. It is then substituted by a collection of many bodies. There exists no sharp border. The value RL is of the order "nm" by a crude estimation for water.

2. Modified Themson-Fermi-Dirac theory of EOS

The total energy of a bulk material is given by [1]

$$E = K + \Phi + \Phi_s \tag{1}$$

where Φ_s is the energy of pseudpotential

$$\Phi_s = -\frac{Q^2}{\varepsilon_0 2R}, \qquad Q = 4\pi R^2 \sigma \tag{2}$$

where σ is the surface charge density. K and Φ are total inner kinetic and potential energy of the bulk, respectively.

On the surface of the bulk there exists a surface tension γ inside electron tunneling through the boundary which form a shell of electrons. It creates a pressure:

$$P_s = \frac{2\gamma}{R} \tag{3}$$

Note that R is radius of the bulk which can be taken as a sphere. Enclosing the bulk is a crust of tunneling electrons with surface charge density σ. A pressure due to extension is thus created:

$$P_\sigma = \frac{(4\pi\sigma)^2}{\varepsilon_0 8\pi} = 2\pi\sigma^2 / \varepsilon_o \tag{4}$$

It follows that eq. (2) can be written as

$$\Phi_s = -3PV = -\frac{Q^2}{\varepsilon_o 2R} \quad (Q = 4\pi R^2 \sigma) \tag{5}$$

in which ε_o is diaelectric constant.

The net pressure on the quantum bag is

$$P_i = P_s - P_\sigma = \frac{2\gamma}{R} - \frac{4\pi\sigma^2}{\varepsilon_o} \tag{6}$$

P_i must be negative, so that the shell of electrons should be stable. Hence,

$$\frac{2\gamma}{R} - \frac{2\pi\sigma^2}{\varepsilon_o} < 0 \ , \qquad R > \frac{\gamma\,\varepsilon_o}{\pi\sigma^2} = R_L \tag{7}$$

If $R < R_L$, the crust of electrons, being referred as "Quantum Bag", will be unstable and another state of electrons inside the bag will be build. This is a nm particle that would resist uniform aggregation. This explains the mechanism of the nm particle that would remain as an individual unit. That is nm water drops remaining in nm size and would not merge into a single bulk.

3. Pressure estimate

Application of the modified TDF theory could provide an estimate of the prevailing pressures by application of the zero pressure (free state) condition. Consider the pressure Pe of the electron on the surface:

$$P_e = \frac{h^2}{5m}\left(\frac{3}{8\pi}\right)^{2/3} n^{2/3} - \frac{1}{4}\left(\frac{3}{\pi}\right)^{1/3} e^2 n^{1/3} \tag{8}$$

where n is the density of electron at surface. The pseudopotential P_σ takes the form

$$P_\sigma = -\frac{2\pi\sigma^2}{\varepsilon_0} = -\frac{Q^2}{3V\varepsilon_0 2R} \tag{9}$$

In the free state, the two aforementioned pressures should balance such that Pe-P_σ =0. This leads to

$$P_\sigma = -P_e = -\left[\frac{h^2}{5m}\left(\frac{3}{8\pi}\right)^{2/3} n^{5/3} - \frac{1}{4}\left(\frac{3}{\pi}\right)^{1/3} e^2 n^{4/3}\right]. \tag{10}$$

4. Shell model of quantum bag: instability and cracking

Long range Coulomb interaction $-2\pi\sigma^2/\varepsilon_o$ gives a negative pressure in the shell while a short range interaction $2\gamma/R$ is related to the surface energy of tunneling electrons. The stability condition gives.

$$R > R_1 = \frac{\gamma\varepsilon_o}{\pi\sigma^2} \tag{11}$$

For a system of molecules with molecule weight M and density ρ, the molecular radius r_o can be written as

$$\frac{4}{3}\pi r_0^3 \cdot \rho = \frac{M}{6.02 \cdot 10^{23}} \quad , \quad r_0 = \left(\frac{M}{8\pi \cdot 10^{23} \rho}\right)^{\frac{1}{3}} \tag{12}$$

Let η be the number of tunneling electrons per molecule with radius r_o. The limit

$$R_L = \frac{\gamma \varepsilon_o}{\pi\left(\frac{e\eta}{\pi r_o^2}\right)^2} > 1.5\text{nm} \tag{13}$$

can be estimated by using the data for water as $\rho=1$, $\varepsilon_o = 88,\ \gamma = 75$ and $\eta < \frac{1}{3}$. Note that R is the limit of size for which the quantum bag is tenable; it is of the right order of magnitude in nm.

Stability is admissible when $\frac{2\gamma}{R}$ is negligible. Pseudopotential Φ_o would enhance the total energy of a solid block. When R<RL, surface and volume energy are comparable. The system attains a new state such that no distinction between boundary and volume energy would exist. A metastable state would result. It breaks down and cracking could prevail. Fracture occurs in the region of imhomogeneity with size R~RL.

With an external pressure is impressed, the condition of stability becomes

$$-P + \frac{2\gamma}{R} - \frac{(4\pi\sigma)^2}{\varepsilon_o 8\pi} < 0 \quad , \quad R_L < 2\gamma / \left(\frac{(4\pi\sigma)^2}{8\pi\varepsilon_0} + P\right) < R \tag{14}$$

For pressure acting on a bulk, the critical size of the bulk should be smaller than the limit size RL. On the contrary, it should be larger, if an external stress is applied. Hence cracking depends on size and pressure that give rise to a nonhomogeneous environment of micro size.

Cracking begins at a metastable state with dimension less than RL; it tends to exist in regions where impurities and disorders prevail.

5. Concluding

For a quantum bag, surface tension tends to expand the shell of tunneling electron cloud while Coulomb force pulls the electron cloud inward. The pulling force should be much larger than that of expansion, the former is responsible for the pseudopotential that gives a negative potential for all electrons inside. Note that $-\frac{\left(4\pi\sigma R^2\right)^2}{\varepsilon_o 2R}$ acts adiabatically, - $\frac{Q^2}{\varepsilon_o 2R}$. It is because the surface structure is quantized such that any small change can occur only adiabatically, leaving the quantization uneffected. That means that Q would be a fixed quantity when volume changes in a EOS.

When the bulk size decreases, the "quantum bag" becomes unstable and could collapes into a many-body system. There would not be a sharp boundary giving rise to a big molecule. Cracking is a transition when stress encounters such a small region where a stable solid serves as state decays into a big molecule of nm scale size.

Reference

[1] K.J. Cheng, S.Y. Cheng, Theoretical Foundation of Condensed Material, Progress in Nature Science, 6(1) (1996) 12-25.