Lipid Molecule of Cells and Mineral Molecules in Volcanos

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Abstract

A statistical thermodynamics is applied to the lipid molecule with and without cisdouble bond for carbon-hydrate chain and the mineral molecules from volcanos. The density of a particular molecule in each subject is given as a function of temperature and molecular weight, so that the relative rates at thermal equilibrium can be estimated. The stability of the lipid bilayer and the depth of the formation of the mineral molecules can be discussed in the cell and the volcanos, respectively.

An additional approach including their environments is suggseted.

1. Introduction

We have long been interested in human being, especially in sickness, since we met deaths of our dear friends by various diseases. When we go back to the origin of him (or her), we naturally come back to that of earth, since then to the universe. The age of the earth is estimated to be 4. 5-6 Gyr, while that of universe is 10-20 Gyr. We all know that volcanos bring occasionally disasters to the human being, and associated many times with earthquakes.

We think that it is important to start with the molecular biology of the cell¹⁾ in order to give an appropriate answer to the cause of sickness for human being. We understood that geothermy²⁾ is related intimately with the origin of earthquakes.

We cannot answer directly the difficult questions pointed out above. We shall instead to touch the relevant problem from statistical thermodynamical approach. Our approach is based on the work of Kolb and Turner³⁾ on The Early Universe. We shall translate

appropriately the method developed there suitable for our purpose. Our subjects are non-relativistic and restricted to high temperature (relative to that for liquid helium). As will be seen, however, the joint use of special relativity with the statistical mechanics is suitable for our purpose.

We think that our approach has a wide applicabilities to the relevant problems. We shall confine ourselves to the limited number of examples, partly, because we have just started to study these subjects and no enough data been available at the time of writing.

We have experienced that many people working in the relevant fields have limited knowledge on them, even they do not have the common languages in their own relevant fields. By these reasons we shall discuss our subjects in a basic elementary manner. In the beginning we planned to discuss an application of a covariant formulation of Boltzmann equation,³⁾ in which an entropy as well as a temperature automatically come in. In order to explain this method to non-experts we need too many pages, so we shall not do it in this note and leave its study for the interested readers.

In Section 2, we shall discuss our statistical mechanical approach, which is based on the number density of the relavant particles in the configuration space appropriate for our application in relation to chemical potential at thermal equilibrium. Section 3 is devoted to the short summary of the structure of cell and way to estimate the ratio of lipids with and without cis-dipole. In Section 4 we shall try to correlate the relative abundance of the observed minerals at certain volcanos in relation to their origins in terms of temperature and depth in the earth.

We think that our approach is somewhat different from usual search of chemical equilibrium, where there appear an defining relation for equilibrium constant from the beginning.⁴⁾

The motives of this work are due to two reasons. We lost our teachers and friends by cancers. We found that the fundamentals for that sickness lie in the study of cells. This is the first try to get familiar with them. The disaster delivered by Fugendake at Nagasaki and its daily activity is reported, but no fundamental understanding is going on as far as an apparent report concerns. Our work is limited to the non-expert approach to understand it from different view.

2. Formalism

We are interested in the molecules at high temperature, so that the Boltzmann statistics is sufficient for their treatment. As is well known that the partition function for the internal motion of the molecule is independent from the volume, viz., density,⁴⁾ we shall take solely into account the translational motion of the center of mass of each molecule.

In this note we consider the relative abundance of molecules with and without certain bond in case of liquid bilayer, and the temperature and production depth of mineral molecules in case of volcano. For both of these problems we start from the number density of a molecule X in phase space, here the energy is assumed to be that given by the special theory of relativity. In this manner the binding energy of the molecule is automatically taken into account.

We shall take the Boltzmann constant $k_B=1$ throughout the paper. In addition to this we choose a natural unit $\bar{h}=c=1$. Under these choices all physical quantities are measured in the unit of energy.^{5),6)} It would be convenient to use eV for our purpose, since 1 eV is approximately 10⁴K.

The number density of a molecule X in the phase space is defined by

$$n_{\mathbf{X}}(\overrightarrow{\mathbf{x}}, \overrightarrow{\mathbf{p}}) = \frac{1}{(2\pi)^3} g_{\mathbf{X}} \exp(-(\mathbf{E}_{\mathbf{X}} - \mu_{\mathbf{X}})/\mathbf{T}, \qquad (2.1)$$

where E_X is the energy of the molecule X including its rest energy, μ_X the chemical potential, T the temperature and g_X the spin statistical weight. The factor $1/(2\pi)^3$ arises from the Fourier transform of the three dimensional delta function, viz.,

$$\delta^{3}(\overrightarrow{p}) = \frac{1}{(2\pi)^{3}} \int e^{-ip \cdot x} d^{3}x. \qquad (2.2)$$

An explicit form of E_x is given in a non-relativistic approximation by

$$E_{X} = \sqrt{M_{X}^{2} + p^{2}} = M_{X} + \frac{p^{2}}{2M_{Y}}, \qquad (2.3)$$

where m_X is the mass of the molecule X and p its momentum. Substituting Eq. (2. 3) into Eq. (2. 1) and integrating over phase space, and after dividing it by the volume V, the number density of X is given by⁷⁾

$$n_{X} = \left(\frac{M_{X}T}{2\pi}\right)^{\frac{3}{2}} \exp(\mu_{X} - M_{X})/T.$$
 (2. 4)

We are interested in the thermal equilibrium for the chemical reaction, e. g.,

$$X + Y \rightleftharpoons A + B + C + \dots \qquad (2.5)$$

where X, Y, A, B, C, ····· are molecules of interests. In a chemical equilibrium we expect to have

$$\mu_{\rm X} + \mu_{\rm Y} = \mu_{\rm A} + \mu_{\rm B} + {}_{\rm C} + \cdots$$

(2.6)

One can define the number densities for molecules Y, A, B, C, analogously for X in (2. 4). Substituting them into Eq. (2. 5) one finds the relative number densities of interests. We shall make an explicit use of the method discussed above in our application.

Before ending this section it would be useful to notice that n_X in Eq. (2. 4) has a dimension of an inverse volume, since the mass and T in our units take the dimension of inverse length. Each of them has simultaneously an energy unit.

3. Lipid Bilayer of Cells

A bilayer form of lipid molecules and protein molecules of about 50% each in membrane structure constitute the so-called plasma membrane.¹⁾ The detail is discussed in Chap. 6 of ref.¹⁾ We shall recommend the reader to look at many figures presented in that book. We shall quote a first statement made in that chapter. "A plasma membrane encloses every cell, defining cell's extent and maintaining the essential differences between its contents and the environment. This membrane is a highly selective filter and a device for active transport; it controls the entry of nutrients and the exit of waste products, and it generates differences in ion concentrations between the interior and exterior of the cell. The plasma membrane also acts as a sensor of external signals, allowing the cell to change in response to environmental cues." It was discussed that why lipid bilayer is formed around cells. Since the head part of lipid molecule is hydrophilic, while its tail is hydro-

Table I Approximate Compositions of Different Cell Membranes*

Percantage of total lipid by wieght

Lipid	liver plasma membrane	erythrone plasma membrane	myelin	mitochon- drion (inner and outer mem- branes)	endoplas- mic reticulum	E. coli
cholesterol	17	23	22	3	6	0
phosphatidyleth- anolamine	7	18	15	35	17	70
phosphatidylserine	4	7	9	2	5	trace
phosphatidylcholine	24	17	10	39	40	0
sphingomyelin	19	18	8	0	5	0
glycolipidis	7	3	28	trace	trace	0
others	22	14	8	21	27	30
total	100	100	100	100	100	100

^{*} This table is taken from Table 6-1 of Alberts et al.¹⁾ We have replaced arbitrarily the number 13 in the last composition for the second item (erythrone plasma membrane) in the original table by 14 in order to make its total 100.

phobic, the lipid molecules together with protein molecules constitute the lipid bilayer. The head side always lies outside of the layer. The six types of typical plasma membranes are listed in Table I with composite percentages of lipids. From the table we see that the first three plasma membranes have more or less similar structure, especially, the first two.

Any operation of cancer of liver is forbidden by the present medical stage, the use of similarity of liver plasma membrane and erythrone plasma membrane in some way will help for medical work. If a lack of some lipid molecules in liver cancer is found the use of other five membranes for its recovery should also be taken into account. This is a qualitative comment seen from the table.

A single bond of carbon hydrate chain in one of the two tails of lipid molecule becomes cis-double bond by taking out two hydrogen atoms. The lipid molecules are bound to the lipid bilayer around a cell. The molecule can change its position with the one of its forward and backward ones and its left and right ones, and sometimes with one at an opposite side of membrane. It is not doing the compeletely free motion. We shall treat it as completely free molecule in the first approximation. If we do this we can apply the method discussed in the previous section for the chemical equilibrium among lipid molecules with and without cis-double and two hydrogen atoms. We can put the all spin weight factors equal to 1 for three different states. Let us consider the following chemical reaction

Here, "none", "cis" and H mean without, with cis-double bond and hydrogen atom, respectively. The chemical equilibrium of reaction (3. 1) is specified by the equality of the associated chemical potentials:

$$\mu_{\rm cis} + 2\mu_{\rm H} = \mu_{\rm none}.$$
 (3. 2)

At a temperature T = 273 + 37 = 310K (approximate value for the human being), one finds then

$$\exp\left(\frac{\mu_{\text{none}}}{T}\right) = \exp\left(\frac{\mu_{\text{cis}} + 2\mu_{\text{H}}}{T}\right). \tag{3.3}$$

Replacing the suffix X in Eq. (2.4) by the appropriate ones in this section and substituting them into Eq. (3.3) one may find

$$\begin{split} n_{\text{none}} \; \left(\frac{2\pi}{M_{\text{none}} T} \right)^{\frac{3}{2}} & \text{exp} \; \left(\frac{M_{\text{none}}}{T} \right) = n_{\text{cis}} \; \left(\frac{2\pi}{M_{\text{cis}} T} \right)^{\frac{3}{2}} & \text{exp} \; \left(\frac{M_{\text{cis}}}{T} \right) \; . \\ & \left(n_{\text{H}} \; \left(\frac{2\pi}{M_{\text{H}} T} \right)^{\frac{3}{2}} & \text{exp} \; \left(\frac{M_{\text{H}}}{T} \right) \; \right)^{2} . \end{split}$$

Rewriting this expression we get

$$n_{cis} = \frac{n_{none}}{n_{H}^{2}} \left(\frac{M_{cis}}{M_{none}}\right)^{\frac{3}{2}} \left(\frac{M_{H}T}{2\pi}\right)^{3} \exp\left(-\frac{B_{none}}{T}\right), \qquad (3.4)$$

where the binding energy for "none" is defined by

$$B_{\text{none}} = M_{\text{cis}} + 2M_{\text{H}} - M_{\text{none}}. \tag{3.4}$$

We shall leave the numerical work for a particular lipid molecule to the reader. We have done a drastic approximation in order to derive Eq. (3.4). If we have a more experience to the real lipid bilayer world, we can improve our approximation suitable to the practical study. In this sense one who has interested in the method discussed here please get contact with us, in order to improve the approach to a more useful one.

4. Igneous Rocks

Before doing any detailed calculation, it is interesting to look at the table of mean chemical composition of main igneous (eruptive) rocks. One finds that relative percentages of twelve oxide compounds for eight main eruptive rocks, due to S. R. Nockolds (1954), are listed in the page 727 of ref.⁸⁾ One sees that all the compounds are oxide ones. We imagine therefore that all of them have had a chance to contact with the underground water before eruption.

The dangerous pyroclastic flows are reported daily from Fugendake of Unzen at Nagasaki. They are associated with vapor. If we once more see the above table, percentage of p_4O_5 is less than 0.4% for all eight rocks. The seven chemical compounds of twelve ones are mono-oxides. The remaining three are SiO_2 , TiO_2 and Al_2O_3 . We imagine that the rocks with a large percentage in association with these three compounds have had big chances to contact with the water during and before the eruption. More explicitly percentage compositions of SiO_2 , Al_2O_3 in calcalkali granite and calcualkali rhyolite are 72.08, 13.86 and 73.66, 13.45, respectively. The percentage of TiO_2 is relatively small for all eight rocks, so we shall omit its role in our first consideration. The total composition rates of SiO_2 and Al_2O_3 in diorite, andesite, gabbro, tholeiitic basalt,

alkaline basalt and peridotite are 68.26, 71.37, 65.20, 64.30, 60.42 and 47.53%, respectively. Comparing these numbers we suppose that the pyroclastic flow will be associated more often with the calcalkali granite and rhyolite type rocks. If this conclusion is not realized in nature, we expect that these rocks have had a chance to meet with water at far deep underground relative to other six rocks. This idea depends, of course, on the volcano. We hope that the crude estimate made here should be checked directly by the existing data.

We have compared the chemical compositions of three mountains, Kilauea, Miharayama and New Showa Mountain,²⁾ with the known eruptive rocks⁷⁾ in Table II, based on the similarity of the composite molecules. The information of these mountains is limited solely on four composites, however, it is instructive to see what we learn from this table.

Table II.	Comparison of	Composions	of Volcanic	and Known	Rocks*	in 9	%
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composition	Kilauea	tholeiitic basalt	Mihara Yama	diorite	New Showa Mountain	calcalkali granite
SiO ₂	50.52	50.23	52.45	51.86	68.89	72.08
FeO	9.77	9.00	10.03	6.97	1.78	1.67
MgO	7.07	6.34	4.62	6.12	0.90	0.52
CaO	11.33	10.42	9.73	8.40	4.10	1.33

^{*} Data on volcanos are taken from introduction of text book by Hayakawa²¹ and those for known rocks from Annual Science Table.¹¹

According to Hayakawa²⁾ the viscosities of eruptive rocks in these mountains are $10^{3.5}$, $10^{5.5}$ and 10^{11} Poise, respectively, at about 1300 K in the corresponding order. If no water is associated the result shows that the pyroclastic flow occurs less often in these osders. This indicates that Si atoms of SiO_2 in New Showa Mountain have had a chance to meet water at rather deep underground relative to that for Kilauea and Miharayama.

The depth-density and depth-temperture relations on earth are given in Fig. 1. 8 and Fig. 1. 12 of ref.²⁾ Unfortunately no separate data for Si are available for the former case. From these figures we learn that the higher the depth the higher density and temperature are required.

We have a number density of SiO₂ from Eq. (2.4) as

$$n_{SiO_2} = \left(\frac{M_{SiO_2}T}{2\pi}\right)^{\frac{3}{2}} \exp(\mu_{SiO_2} - M_{SiO_2})/T$$
 (4. 1)

which means that the high T is required in order to produce a high density n_{SiO_2} .

A similar argument applies to all other molecules.

It is too impatient to require a quick conclusion from a limited information. We need a more information on a water system on the surface of the earth, especially for the pyroclastic flow, in order to give a definite answer on a specific volcano.

5. Discussion

We have discussed the lipid molecule with and without cis-double bond and the molecules in the eruptive rocks for volcano as illustrations. Our idea discussed in Section 2, however, has wider applicabilities for many chemical reactions, owing to its generality. Perhaps a more interesting application will be the chemical reaction between those in cell and medicine through lipid bilayer, where one can discuss how to cure ill cells.

For the sake of defniteness, let us confine ourselves to three to two molecule reaction for Eq. (2.5), viz., from A+B+C to X+Y. For simplicity we assume that the lipid bilayer is working normally. Suppose that the molecules A, B and C are members of ill cell, of medicine and water one. The X and Y are cured molecule and a product one after the recovery of the cell, which will be exited through plasma membrane as discussed by Alberts et al.¹⁾ We leave a detailed examination of many analogous problems to the reader.

We cannot say much about pyroclastic flow at Fugendake, since we do not have any data from molecular approach. We hope that such an investigation in comparison with the existing data on other volcanos will help us both for present and future study.

We have shown a startistical thermodynamic approach by confining to both limited theory and fields of science. If the situation admits us to work further we may willing to do so.

Acknowledgement

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- 1) B. Alberts, D. Bray, J. Lewis, M. Raff, K. Roberts and J. D. Watson, Molecular Biology of The Cell, 2nd Ed., (Garland Pub., 1989).
- 2) M. Hayakawa, Geothermy, in Japanese (Tokai Univ. Pub., 1988).
- 3) E. M. Kolb and K. E. Turner, The Early Universe (Addison-Wesley, 1990).
- 4) T. M. Reed and K. E. Gubbins, Applied Statistical Mechanics (Butterworth-Heinemann, 1973).
- 5) A detailed explanation of the natural units is given in ralation to classical electrodynamics. 6) Once one has practiced to use them he can understand their universal applicability to any field of science.
- 6) S. Iwao, Introduction to Physics (III) Mainly Electromagnetism and Differential Geometry, in Japanese (Kanazawa Univ. Press, 1988).
- 7) One cannot perform the integration suggested is recommended to read S. Iwao, Introduction to Physics (II) Mainly Theory of Vibration and Statistical Thermodynamics, in Japanese (Kanazawa Univ. Press,1987), 2nd Ed. Here the mathematics necessary for Bose and Fermi statistics associated with the chemical potential have also been discussed in detail. If one feels a difficulty to read Chap. 1 of ref.²⁾ He is recommended to look at above text.
- 8) Annual Scince Table, Edited by National Astronomical Observatory, in Japanese, Nov. (Maruzen, 1991).