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Inevitability of Spiral-shape in DNA

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Abstract: Cyto-fluid dynamic theory, which clarifies the inevitability of the size ratio of purine and pyrimidine in the base-pairs, is extended to reveal the inevitability of the spiral-shaped double-strand of bases-pairs, i.e., DNA. First, we will define the cluster consisting of a nitrogenous base and water molecules as continuum flexible particle. Then, momentum conservation law and quasi-linear stability theory clarifies the inevitability of spiral shape of B-DNA.

Keywords: DNA, water, inevitability, cyto-fluid dynamic theory

I. INTRODUCTION

Molecular biology, started by Watson, Crick, and Franklin, has solved some important mysteries related to heredity and self-replication. However, concurrently, the clarification of DNA and RNA structures brought us new mysteries.

One is why living beings use only five types of nitrogenous bases and twenty types of amino-acids. We explain the inevitability of these molecules by proposing the fluid-dynamic theory. [1, 2, 3] Inevitability of the clover shapes in tRNA and rRNA is also clarified by continuum mechanics. [2, 3, 5]

The other mystery will be related to macroscopic structures such as cells and organs. The researches on the structures of cells and brain [4, 5, 6] are also done with fluid-dynamics, which keep a distance from previous reports based on informatics and mathematics [7, 8]. However, there are still a lot of mysteries related to bio-structures. Here, we will reveal one of the key mysteries between micro- and macro-structures, inevitability of spiral shape of B-DNA.

II. CYTO-FLUID DYNAMIC THEORY [1,2,3]

We can classify five bases of adenine (A), guanine (G), cytosine (C), thymine (T), and uracil (U) into two groups, purine and pyrimidine. Purines, i.e., A and G, have relatively large size, while pyrimidines, i.e., C, T, and U, are small.

In our previous reports, we clarify the reason of why two types of bases (relatively larger purine and smaller pyrimidine) are used in DNA and RNA. [1, 2, 3]

First, we will consider two nitrogenous bases, a purine and a pyrimidine, connected by hydrogen bonds in a large quantity of water. Owing to the influence of the nitrogenous bases, water molecules around the bases have different densities and arrays in comparison with those far away. Thus, we divide the water into two regions. Accordingly, an aggregation of a nitrogenous base and water molecules surrounding it can be treated as a continuum particle such as a transmutable spheroid. (See Fig. 1.) We call this particle as parcel. Then, the flow inside the particle is assumed to be potential one, while there is tension at the particle surface. (See Eq. 1.)

$$\Delta\phi = \frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2} \tag{1}$$

Based on these assumptions, we previously derived a deterministic momentum equation describing particle deformation. When a small disturbance is given for two connected flexible particles, the deformation rate ξ of each particle dependent on time t can be described as

$$d^2\xi/dt^2 = (\varepsilon - 1)(d\xi/dt)^2 + (\varepsilon^3 - 3)\,\xi \tag{2}$$

where parameter ε denotes the size ratio of the two particles connected at the equilibrium condition. When the particles are spheres at the equilibrium condition, ξ is zero. A symmetric ratio of 1.0 and an asymmetric ratio of $\sqrt[3]{3}$ around 1.5 make the right-hand side of Eq. (2) zero, which appears as the n-th root of n with n = 1 and n = 3, respectively. The deformation speed is smaller for ε = 1.0 and $\sqrt[3]{3}$ than for the other values of ε. Life is relatively stable, when the size ratio of hydrogen-bonded nitrogenous bases takes the n-th root of n, which has the values of 1.0 and 1.44 for n=1 and 3, respectively.

The quasi-stability maintains the hydrogen-bonded pairs of two identical bases and of purine-pyrimidine over a period of time. (Pairs of two identical bases can be often seen in RNA, while purine-pyrimidine pairs are rich in RNA and DNA.)

Figure 1 assumes that water molecules around base are dense. However, even if water molecules around base are less, i.e., hydrophobic, two particles connected are quasi-stable at e = 1.0 and $\sqrt[3]{3}$.

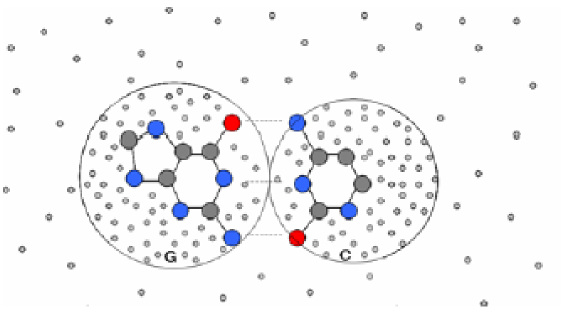

Fig. 1. Two hydrogen-bonded purine and pyrimidine bases surrounded by water molecules.

II. DNA

It is well-known that the weight of hydrated water molecules per a base-pair inside DNA is of the order of that of the bases-pair. [12-15] Thus, we assume that the base-pairs inside DNA can also be modeled by flexible parcels shown above. Only one difference from the foregoing section is that the flexible parcel is redefined as a column having the cross-section of ellipsoid (Fig. 2 and Eq. 2), which possesses spiral-shaped axis at the center. (See Fig. 3. Center line of the column is not straight, curved like spiral.)

$$\frac{(x - X_s + a)^2}{a^2} + \frac{y^2}{b^2} = 1 \tag{3}$$

where a and b denote time-dependent radii of the ellipsoid. Equivalent radius of the ellipsoid rd satisfies $r_d^2 = ab$.

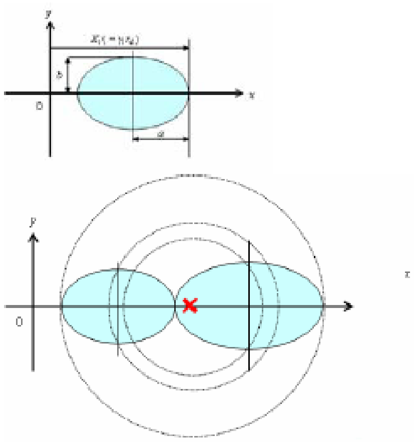

Fig. 2 Column having the cross-section of ellipsoid.

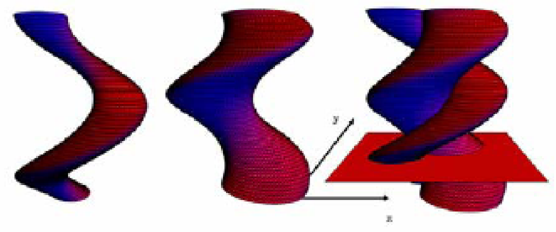

Fig. 3 Columns for double-strand DNA.

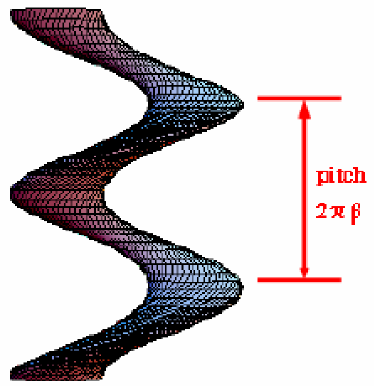

Fig. 4 Pitch of spiral

Figure 4 demonstrates the pitch of spiral in single column divided by 2π, β. Quantity δ denotes dimensionless pitch defined by

$$\delta = \frac{\beta}{r_{d1} + r_{d2}} \tag{4}$$

where r_{d1} and r_{d2} denote the equivalent radii of two ellipsoids connected. Double strand system shown in Fig. 3(c) models the DNA, where the ratio of two radii ε is defined by

$$\varepsilon = \frac{r_{d1}}{r_{d2}} \tag{5}$$

Then, the dimensionless deformations of two ellipsoids connected are denoted by

$$\gamma_1 = a_1 / b_1 \ and \ \gamma_2 = a_2 / b_2 \tag{6}$$

Assumptions based on Eqs. (1), (3), (4), (5) and (6) leads us to the following momentum conservation law.

$$\frac{d^2\gamma_1}{dt_1^2} = \frac{\left\{\begin{array}{l} \left[\left(-1-\varepsilon^2+\frac{1}{2}E_2\gamma_2^{-\frac{1}{2}}\right)B_1+\frac{1}{4}\varepsilon^2 E_1\gamma_1^{-\frac{3}{2}}\right]\left(\frac{d\gamma_1}{dt_1}\right)^2 \\ +\varepsilon^2 E_1\left(\frac{1}{2}B_2\gamma_2^{-\frac{1}{2}}-\frac{1}{4}\gamma_2^{-\frac{3}{2}}\right)\left(\frac{d\gamma_2}{dt_2}\right)^2 \\ +\left(-1-\varepsilon^2+\frac{1}{2}E_2\gamma_2^{-\frac{1}{2}}\right)C_1+\frac{1}{2}\varepsilon^2 E_1\gamma_2^{-\frac{1}{2}}C_2 \end{array}\right\}}{DET}$$

$$\frac{d^2\gamma_2}{dt_2^2} = \frac{\left\{\begin{array}{l} E_2\left(\frac{1}{2}B_1\gamma_1^{-\frac{1}{2}}-\frac{1}{4}\gamma_1^{-\frac{3}{2}}\right)\left(\frac{d\gamma_1}{dt_1}\right)^2 \\ +\left[\left(-1-\varepsilon^2+\frac{1}{2}\varepsilon^2 E_1\gamma_1^{-\frac{1}{2}}\right)B_2+\frac{1}{4}\varepsilon^2 E_2\gamma_2^{-\frac{3}{2}}\right]\left(\frac{d\gamma_2}{dt_2}\right)^2 \\ +\frac{1}{2}E_2\gamma_1^{-\frac{1}{2}}C_1+\left(-1-\varepsilon^2+\frac{1}{2}\varepsilon^2 E_1\gamma_1^{-\frac{1}{2}}\right)C_2 \end{array}\right\}}{DET}$$

$$DET = -1-\varepsilon^2+\frac{1}{2}\varepsilon^2 E_1\gamma_1^{-\frac{1}{2}}+\frac{1}{2}E_2\gamma_2^{-\frac{1}{2}}$$

$$w_1^2 = \frac{8\sigma}{\rho_L r_{d1}^3}$$

$$w_2^2 = \frac{8\sigma}{\rho_L r_{d2}^3}$$

$$t_1 = w_1 t$$

$$t_2 = w_2 t \tag{7}$$

where the constants in Eq. (7) are as follows.

$$B_1 = \frac{\gamma_1^2-3}{2\gamma_1\left(\gamma_1^2-1\right)}$$

$$B_2 = \frac{\gamma_2^2-3}{2\gamma_2\left(\gamma_2^2-1\right)}$$

$$C_1 = \frac{\gamma_1^2}{2\left(\gamma_1^2-1\right)}\left(\begin{array}{l} \gamma_1^{\frac{3}{2}}-\gamma_1^{-\frac{3}{2}} \\ +\frac{(\gamma_2^{\frac{1}{2}}-\varepsilon\gamma_1^{\frac{1}{2}})\{\gamma_1^{\frac{3}{2}}(\gamma_2^{\frac{1}{2}}-\varepsilon\gamma_1^{\frac{1}{2}})+\varepsilon\}}{(1+\varepsilon)^2\delta^2} \\ -\varepsilon^2(1+\varepsilon)\delta\frac{\gamma_1^{-\frac{3}{2}}(\gamma_1-\gamma_1^{-1})}{\{\gamma_2+(1+\varepsilon)^2\delta^2\}^{\frac{3}{2}}} \end{array}\right)$$

$$C_2 = \frac{\gamma_2^2}{2\left(\gamma_2^2-1\right)}\left(\begin{array}{l} \gamma_2^{\frac{3}{2}}-\gamma_2^{-\frac{3}{2}} \\ +\frac{(\varepsilon\gamma_1^{\frac{1}{2}}-\gamma_2^{\frac{1}{2}})\{\gamma_2^{\frac{3}{2}}(\varepsilon\gamma_1^{\frac{1}{2}}-\gamma_2^{\frac{1}{2}})+1\}}{(1+\varepsilon)^2\delta^2} \\ -(1+\varepsilon)\delta\frac{\gamma_2^{-\frac{3}{2}}(\gamma_2-\gamma_2^{-1})}{\{\varepsilon^2\gamma_1+(1+\varepsilon)^2\delta^2\}^{\frac{3}{2}}} \end{array}\right)$$

$$E_1 = 4\frac{\gamma_1^{\frac{5}{2}}}{\gamma_1^2-1}$$

$$E_2 = 4\frac{\gamma_2^{\frac{5}{2}}}{\gamma_2^2-1}$$

Finally, we will get the first-order of approximation for Eq. (7), while small deformations for ellipsoids are put. (See Eq. 8.)

$$\frac{d^2\xi_1}{dt_1^2} = B_{11}\left(\frac{d\xi_1}{dt_1}\right)^2+B_{12}\xi_1+B_{13}\left(\frac{d\xi_2}{dt_2}\right)^2+B_{14}\xi_2$$

$$\frac{d^2\xi_2}{dt_2^2} = B_{21}\left(\frac{d\xi_1}{dt_1}\right)^2+B_{22}\xi_1+B_{23}\left(\frac{d\xi_2}{dt_2}\right)^2+B_{24}\xi_2 \tag{8}$$

where small deformations $\xi 1$ and $\xi 2$ satisfy $\gamma 1= k1+\xi 1$ and $\gamma 2=k2+\xi 2$, with dimensionless radii at equilibrium k1 and k2, respectively.

III. RESULTS

In the previous reports [1,2,3], we propose the concept of quasi-stability, which is weaker than neutral stability. Quasi-stability implies that the system is relatively stable for initial disturbances. For example, if each term in the right hand sides of Eq. (8) become zero, the number of terms which have influence of disturbances on deformations relatively is reduced. In this sense, the system is relatively stable for the initial stage. Equation 8 brings us the relations between size ratio ε and pitch of spiral δ, with which the spiral shape is quasi-stable. (See Fig. 5.) Predictions of quasi-stable pitch calculated by Eq. (8) agree with actual pitch of B–DNA in life [11].

It should be stressed that Eq. (8) and Fig. 5 show another quasi-stable pitch, which may correspond to A-DNA and C-DNA qualitatively.

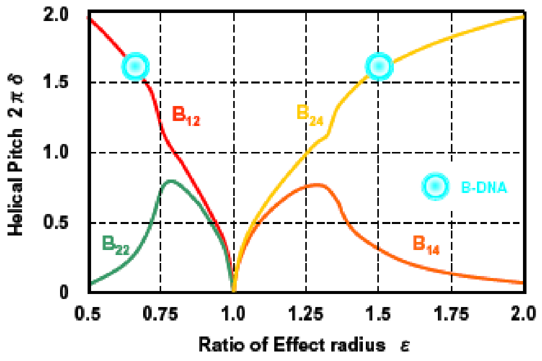

Fig. 5 Quasi-stable helical pitch plotted against size ratio ε.

IV. CONCLUSION

C. R. Calladine and H.R. Drew [11] explain the inevitability of spiral shape of DNA on the basis of chemistry. However, DNA can not take the structure of B-DNA, if there are no water molecules around nucleic acids. Inevitability of spiral shapes of DNA should be explained by considering water molecules around DNA.

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