

## On a Possible Mechanism of the Effect of Microwave Radiation on Biological Macromolecules

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**Abstract**—A model that describes the dissociation of a hydrogen bond in water clusters when irradiated by an electromagnetic field in the microwave range is proposed. The model is also applicable for the case of the rupture of the covalent bond of the water molecule in a cluster. If the energy absorption occurs at the interface of water and polymer clusters (e.g., DNA and chitosan), degradation of the polymer chain is possible.

**Keywords:** water clusters, microwave radiation, mathematical simulation

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Experiments that elucidate the role of the microwave effect in contrast to the thermal effects upon exposure of microorganisms to super-high-frequency (SHF) electromagnetic radiation are classified as controlled temperature and dry experiments. The experiments of the first type did not provide a reliable result [1, 2], while water was found to play an important role in the biocide effects of microwaves in the experiments of the second type [3]. Since water is the initial medium that mediates the transformation of microwaves into heat and DNA has a dielectric dispersion at sufficiently lower frequencies than water, it was concluded in [3, 4] that water mediates the transfer of the thermal energy in a biological system.

Later, DNA fragmentation, which was not observed during external heating up to temperatures that are achieved upon exposure to microwave irradiation, was reliably found in experiments with the exposure of viral DNA to microwave irradiation in an aqueous medium [5]. It is natural that due to energetic reasons the destruction of a chemical bond is difficult to observe during direct irradiation of DNA, since the energy of a microwave photon is approximately  $10^{-5}$  eV, while the dissociation of a covalent bond requires an energy of up to 10 eV, i.e., a million times greater. Thus, these works reliably indicate that water plays an important role in DNA destruction. Experimental studies of the impact of microwave radiation on water revealed three effects: an increase in the optical den-

sity in the near ultraviolet region, the displacement of the chemical shift of a proton toward a strong field, and an increase in the time of spin-lattice relaxation for irradiated water in contrast to water that was not irradiated [6]. All these results are evidence of changes in the cluster structures of water that are connected with breakage of a hydrogen bond. Simulation of 57 and 60 molecular water clusters revealed that the eigenfrequency spectrum of these formations is within the millimeter and submillimeter ranges [7], which makes it possible to propose resonance absorption of microwave radiation for these formations.

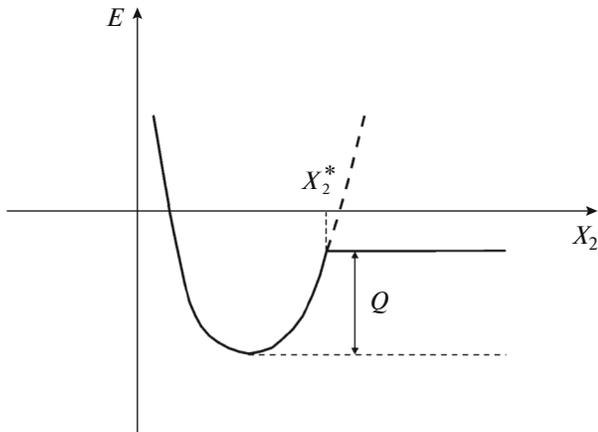
In this case, a peculiar effect is possible, viz., the energy of the electromagnetic oscillations could be absorbed at the eigenfrequencies of cluster oscillations, which due to van der Waals forces transfer the excitation energy to the oscillations of the hydrogen and chemical bonds. Thus, water clusters are nanomediators of the thermal effect of microwaves.

### MODEL

We attempted to create a simple microscopic model of the destruction of a chemical bond under the effect of electromagnetic radiation at relatively low frequencies that occurs via water nanomediators.

The anharmonicity in crystals and large molecules is known to lead to the presence of highly excited localized vibrational states that are different from the states of linear systems [8]. The physics of these processes is reduced to the fact that at large amplitudes of the excitation of one oscillator the frequencies of two

*Abbreviations:* SHF, super-high-frequency.



The potential energy for a fast harmonic oscillator. Dissociation of a chemical bond occurs when the oscillator coordinate is reached.

weakly interacting oscillators vary considerably, since the eigenfrequency of an anharmonic oscillator depends on its amplitude. This results in a disturbance of the resonance and low probability of the energy transfer from one oscillator to another. An alternative system for the presence of these local modes is a system of two interacting anharmonic oscillators with different oscillation frequencies, with one of them resonantly interacting with an external periodic field. Water can represent this system in the real world [6, 9]. At the interphase boundaries (in the “water–biological object” system) water clusters form a certain order; here, all the clusters vibrate at the same frequency by acquiring a common frequency [6, 7]. The frequency of the cluster oscillation at room temperature of 18°C is  $6.79 \cdot 10^9$  Hz [10]. Under the effect of an electromagnetic field at a close frequency the cluster is excited and the amplitude of the oscillations becomes greater. Upon weak interaction with normal oscillations of atoms in the cluster, this state with the local mode exists for a sufficiently long period. Therefore, the time of this complete energy transfer without exchange from one oscillator to another increases. This situation is described mathematically by the system of two equations

$$\begin{cases} \ddot{X}_1 + \gamma_1 \dot{X}_1 + \Omega_0^2 X_1 + \lambda X_1^3 = \frac{\beta}{M} X_2 + \frac{F_0}{M} e^{i\omega t}, \\ \ddot{X}_2 + \gamma_2 \dot{X}_2 + \omega_0^2 X_2 + \lambda X_2^3 = \frac{\beta}{\mu} X_1. \end{cases} \quad (1)$$

Here,  $X_1$  and  $X_2$  are the coordinates of the first and second oscillators;  $\Omega_0$  is the zero frequency of the first oscillator;  $\omega_0$  is the zero frequency of the second oscillator;  $\omega$  is the frequency of the external electromagnetic field;  $\lambda$  and  $\beta$  are parameters that describe

anharmonicity and bonding force of the both oscillators, respectively;  $M$  and  $\mu$  are the masses of the first and second oscillators, respectively; and  $F_0$  is the amplitude of the force of the external field.

Taking the fact that  $M \gg \mu$  into account and neglecting the anharmonicity term of the both oscillators and their attenuation, we simplify the problem by simulating a system that contains two harmonic oscillators

$$\begin{cases} \ddot{X}_1 + \Omega_0^2 X_1 = \frac{F_0}{M} e^{i\omega t}, \\ \ddot{X}_2 + \omega_0^2 X_2 = \frac{\beta}{\mu} X_1. \end{cases} \quad (2)$$

We solve this system of equations for two cases: (1) in the general case, when the frequency of the first oscillator does not coincide with that of the external field, i.e.,  $\Omega_0 \neq \omega$ , the system of two second-order nonhomogeneous differential equations is solved by the Green-function method [11] and (2) upon resonance interaction of the first oscillator with the external field, i.e.,  $\Omega_0 = \omega$ .

(1) In the general case, at  $\Omega_0 \neq \omega$  solving the system of equations at the external field  $F(t) = F_0 \cos \omega t$  leads to the following expression for the coordinate of the second oscillator

$$X_2 = \frac{F_0 \beta}{M \mu \omega_0^2 (\omega^2 - \Omega_0^2)} [\cos \Omega_0 t - \cos \omega t]. \quad (3)$$

We assume that at  $t = \tau^*$  the amplitude of the oscillations of the second oscillator is such that the energy of the oscillator is equal to the dissociation energy  $Q$  (Fig. 1). The equation then can be rewritten as

$$\begin{aligned} X_2^* &= \frac{F_0 \beta}{M \mu \omega_0^2 (\omega^2 - \Omega_0^2)} \\ &\times [\cos \Omega_0 \tau^* - \cos \omega \tau^*] = \sqrt{\frac{2Q}{\omega_0^2 \mu}}. \end{aligned} \quad (4)$$

By rearranging the constants on one side of the equation, we obtain

$$\cos \Omega_0 \tau^* - \cos \omega \tau^* = \frac{M \omega_0 (\omega^2 - \Omega_0^2)}{F_0 \beta} \sqrt{2Q\mu} \leq 2. \quad (5)$$

The parameters from this equation that correspond to the case of microwave irradiation of water clusters and rupture of a hydrogen bond [8, 10] can possess the following values

$$\begin{aligned} \Omega_0 &= 6.79 \cdot 10^9 \text{ Hz}, \quad \omega_0 = 5 \cdot 10^{13} \text{ Hz}, \quad \omega = 7 \cdot 10^9 \text{ Hz}, \\ M &= 57(m_O + 2m_H) = 57 \cdot 3 \cdot 10^{-23} \text{ g} = 1.71 \cdot 10^{-21} \text{ g}, \\ \mu &= m_H = 0.167 \cdot 10^{-23} \text{ g}, \quad \text{and } Q = 25 \text{ kJ/mol}. \end{aligned}$$

The maximum difference between cosines is two, which corresponds to the minimum values of the coupling constant and amplitude of the force of the external field. The amplitude of the force of the external field can be calculated based on the field strength at the intensity of an SHF field of  $I \sim 10^{-3}$  W/cm<sup>2</sup>. The strength of the electromagnetic field is calculated from the equation  $E \approx 20\sqrt{I}$  and is 1.57 V/cm. Then,  $F_0 = 2.5 \cdot 10^{-7}$  N and  $\beta = 20$  kg/s<sup>2</sup>  $\approx 1$  eV/A<sup>2</sup>.

By solving the equation at the given values of the parameters we could assess the time  $\tau^* \approx 1.5 \cdot 10^{-8}$  s, which corresponds to the time of accumulation of energy on the second oscillator that is sufficient for dissociation of a hydrogen bond. In the case of the rupture of a chemical bond,  $Q$  and  $\beta$  will be different.

(2) In the case of the resonance interaction of the first oscillator with the external field, i.e., when  $\Omega_0 = \omega$ , system of equations (2) can be written as

$$\begin{cases} \ddot{X}_1 + m^2 X_1 = a \sin mt, \\ \ddot{X}_2 + \omega_0^2 X_2 = \frac{\beta}{\mu} X_1, \end{cases} \quad (6)$$

where  $m = \omega = \Omega_0$  and  $a = F_0/M$ .

By solving this system of equations [11], we obtain for the coordinate of the second oscillator

$$\begin{aligned} X_2 \approx & \frac{F_0 \beta}{M m \mu} \left[ -\frac{2m}{\omega_0^4} [\cos mt - \cos \omega_0 t] \right. \\ & \left. + \frac{1}{\omega_0^3} [\sin mt - \sin \omega_0 t - \omega_0 t \sin mt] \right]. \end{aligned} \quad (7)$$

In this case, the time  $\tau^*$  that is necessary for bond dissociation also can be calculated based on Eq. (4). The estimates of these expressions demonstrate that  $\tau^*$  in the second resonance case is approximately  $10^{-8}$  s and insignificantly differs as compared to the first case.

(3) It is of particular interest to compare the discussed mechanism of energy transfer of the energy of the SHF field via a water cluster with the channel of an increase in the vibrational energy of the fast oscillator at its immediate interaction with an SHF field that has the frequency  $\omega$ , which corresponds to the case of SHF irradiation of a macromolecule without water. Then, the motion equations for the fast oscillator are [12]

$$\ddot{X}_2 + \omega_0^2 X_2 = \frac{F_0}{\mu} e^{i\omega t}. \quad (8)$$

The solution of this equation under the initial conditions  $t = 0, X_2 = \dot{X}_2 = 0$  is

$$X_2 = \frac{F_0}{\mu(\omega_0^2 - \omega^2)} \cos \omega t. \quad (9)$$

Then, the condition of dissociation of a chemical bond during the time  $\tau^*$  is the following

$$Q = \frac{1}{2} \omega_0^2 \mu X_2^2 = \frac{1}{2} \frac{F_0^2}{\mu \omega_0^2} \cos^2 \omega \tau^*. \quad (10)$$

Substitution of the parameters  $Q, F_0, \mu,$  and  $\omega$  from paragraph 1 demonstrates that  $Q \gg \frac{1}{2} \frac{F_0^2}{\mu \omega_0^2}$ , i.e., bond rupture during direct excitation of the fast oscillator is impossible. This results is in complete agreement with an experiment on the effect of an SHF field on dry DNA [3].

## CONCLUSIONS

A simplified theoretical model that describes dissociation of a hydrogen bond in water clusters under exposure to an electromagnetic field within a microwave range is proposed. The proposed model could be theoretically applied for the case of the rupture of the covalent bond of a water molecule in a cluster. If the energy absorptions occurs at the interphase boundary of water clusters and a polymer (e.g., DNA or chitosan) then the destruction of the polymer chain is also possible. The special role of a phase interface and hydration shell of macromolecules has been noted in a number of studies [13–15]. Structuring of water-containing media at their contact with materials that include micro- and nanosized inhomogeneities in the contact surface has been observed. It has been demonstrated that structuring of water layers appears to be an essential condition of the observed effects during the interaction of low-intensity microwave radiation with water media, including the biological effects that are used in modern biomedical technologies.

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