

Analysis of Dipole Relaxation Time for Water Molecules at Temperature of 293⁰K

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Abstract

The study of dipole relaxation time for water molecules at 293⁰K is an important aspect from physics / communication / electronic engineering point of view since it gives rise to the dielectric absorption losses for r.f. fields up to about 3×10^{10} Hz of frequencies. Here molecular (dipole) relaxation time is analyzed and calculated for the water molecules at temperature of 293⁰K. This assumes that the water medium is an intermediate one to a solid state and a gaseous state. The molecule of the water undergoes coupled mass vibrations on one hand and simultaneously it has an average thermal velocity on other hand as given by the kinetic theory of gasses. In other words, this is a quasi-stationary: quasi moving system of the molecules, where molecule-molecule collisions take place which are described by gas kinetics. The expression which is obtained for the molecular collision frequency, determines the dipole relaxation time coming in the picture of relaxation spectrum in r.f. region for the water molecules. The present theory given here determines fairly well the value of dipole relaxation time for water at temperature of 293⁰K, viz., the relaxation time is experimentally located near the free space wavelength of 1 cm in the relaxation spectrum of water. Purpose of this work is to show in a simple manner, how dipole relaxation time for water molecules at 293⁰K comes in the analysis of scattering of the dipoles at collisions with each other.

Keywords

Water, Coupled-Mass-Vibrations, Molecule-Molecule, Collisions, Dipole-Relaxation, 293⁰K

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1. Introduction

The study of dipole relaxation time for water molecules at 293⁰K (where ⁰K is Degree Kelvin) is an important aspect from physics/communication/electronic engineering point of view since it gives rise to the dielectric absorption losses for r.f. fields up to about 3×10^{10} Hz of frequencies. This property is useful in microwave heating for microvan-oven for cooking food etc.

Now consider a neutral system of water molecules having N_w molecules per unit volume of it near room temperature (~ 293 ⁰K). Here the water is considered as pure. The water here under consideration is of macroscopic dimensions. Each molecule of the water is associated with a permanent dipole

moment of magnitude μ . These molecules of the water are known as polar molecules. In the absence of an applied r.f. electric field to the water, there is no preferred direction for the dipole moments, and as such the vector sum of all the μ s in any direction is zero, meaning thereby the dipoles are thermally oriented randomly in the water near room temperature (~ 293 ⁰K).

When the water is subjected to a r.f. electric field, then the (permanent) dipoles experience a torque and tend to align (with a slight preferential orientation) in the direction of (which is parallel to) the field for the normal case of (laboratory) field(s) near room temperature (~ 293 ⁰K), against their original (thermal) random orientation as mentioned above, and this produces a polarization termed as orientation polarization, for instance refer to Von Hippel (1954

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pp. 38) [1] and Dekker (1961, Secn. 3.4) [2]. Here for General reference refer also to Stark 1914 [3], Debye 1945 [4], Fröhlich 1949 [5] and Cole and Cole 1941 [6], Buchnen, Barthel, Stauber 1999 [7], Thakur and Singh 2008 [8] and Zasetsky 2011 [9].

When the field is switched on, then dipoles would not simultaneously tend to orient in alignment with the field. A time measure of the dipoles for tending to orient in alignment of them with the field against their original random orientation, is the dielectric relaxation time τ_o . The dipole relaxation time τ_o for the water molecules, is defined as the time required for the dipoles to orient in such a way that the polarization increases to $[1 - (1/\exp)]$ of its final value in the presence of the field (where 'exp' is the base of natural logarithm). In the definition of τ_o , it is assumed that the polarization grows exponentially with time t (measured from the instant when the field is switched on), as follows:

$$P(t) = P(\infty)[1 - \exp(-t/\tau_o)]. \quad (1)$$

Here $P(t)$ is the polarization at time t , and $P(\infty)$ is the final value of the polarization.

Equation (1) suggests that the differential equation for the (growth of) orientation polarization is of the form given by,

$$\frac{\partial}{\partial t} [P(t)] = -\frac{1}{\tau_o} [P(t) - P(\infty)]. \quad (2)$$

Considering the r.f. electric field of instantaneous value $E=E_o \exp(i\omega t)$, where E_o is the peak value of the electric field, ($\omega=2\pi f$ is the angular frequency of the field, f is the frequency of the field, t is the instantaneous time and $i = \sqrt{-1}$), which is applied to the system of dipoles of the water molecules. The value of $P(\infty)$ is given by,

$$P(\infty) = \epsilon_o(\epsilon_r - 1) E_o \exp(i\omega t), \quad (3)$$

where ϵ_r is the relative static permittivity of water with respect to free space [for water here near room temperature (~ 293 °K), ϵ_r is near about 80 (Clark, 1988, pp. 66) [10] and ϵ_o is the permittivity of free space. Here it is considered that, it is ϵ_r which contribute to $P(\infty)$ in eqn. (3), while dealing with the application of r.f. electric field to the system of dipoles of the water molecules. Using eqn. (3), eqn. (2) gives that,

$$\frac{\partial}{\partial t} [P(t)] = -\frac{1}{\tau_o} [P(t) - \epsilon_o(\epsilon_r - 1)E_o \exp(i\omega t)]. \quad (4)$$

Let the steady state solution of eqn. (4), be given by,

$$P(t) = \epsilon_o(\epsilon_r^* - 1)E_o \exp(i\omega t), \quad (5)$$

where ϵ_r^* is the relative complex r.f. dielectric constant of the water with respect to free space. Substituting eqn. (5) in eqn. (4), and solving gives that,

$$\epsilon_r^* = 1 + \frac{\epsilon_r - 1}{1 + i\omega\tau_o}. \quad (6)$$

Here

$$\epsilon_r^* = \epsilon_r' - i\epsilon_r'', \quad (7)$$

where ϵ_r' is the relative r.f. permittivity of the water with respect to free space and ϵ_r'' is the relative r.f. loss factor of the water with respect to free space. Further eqn. (6) on using eqn. (7), and separating the real and imaginary parts of the resultant expression gives that,

$$\epsilon_r' = 1 + \frac{\epsilon_r - 1}{1 + \omega^2\tau_o^2}, \quad (8)$$

and

$$\epsilon_r'' = \frac{\omega\tau_o(\epsilon_r - 1)}{1 + \omega^2\tau_o^2}. \quad (9)$$

The variations of the parameters $(\epsilon_r' - 1)/(\epsilon_r - 1)$ and $\epsilon_r''/(\epsilon_r - 1)$ with angular frequency ω of the r.f. field are shown as in Fig. 1. Both these parameters depend on the product $\omega\tau_o$. Here eqn.(8) and (9) are considered to hold good in the r.f. region of the spectrum of the electromagnetic waves up to a minimum of about 8 mm of the free space r.f. wavelength [for the water near room temperature (~ 293 °K)].

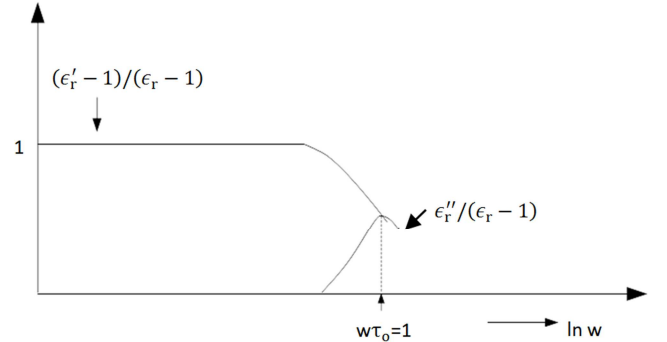


Fig. 1. (Theoretical) plot of $(\epsilon_r' - 1)/(\epsilon_r - 1)$ and $\epsilon_r''/(\epsilon_r - 1)$ versus (logarithm of) angular frequency ω of the r.f. electric field, for water at temperature of 293 °K.

At $\omega\tau_o = (2\pi f)\tau_o = 1$, $(\epsilon_r' - 1)/(\epsilon_r - 1)$ reduces approximately to half the initial value of $(\epsilon_r' - 1)/(\epsilon_r - 1)$, where $\epsilon_r \gg 1$. For $\omega\tau_o > 1$, it decreases down to low values further.

The variation ϵ_r'' depends on the factor $\omega\tau_o/(1 + \omega^2\tau_o^2)$ which has a maximum at $\omega\tau_o = (2\pi f)\tau_o = 1$.

Experimentally, the value of $\omega\tau_o = (2\pi f)\tau_o = 1$ (for example, as that given in Fig. 1) occurs when f corresponds to a free space wavelength which is located near 1 cm in the spectrum of r.f. waves (Von Hippel, 1954, pp. 38) [1] for water near room temperature (~ 293 °K).

Here the dielectric absorption losses due to ϵ_r'' in presence of the r.f. electric field, causes an increase in temperature of the water [which is due to the slight preferential alignment of the

dipoles against their original random orientation, now in the steady state] accounting for the heat losses {for the dielectric losses, refer to Dekker (1961, sec.3.5)[2]}. And a temperature $T = 293^{\circ}\text{K}$ in the present analysis gives an average temperature attained by the water in presence of these heat losses relative to surroundings in equilibrium conditions.

Molecular interpretation of the relaxation time of water molecules, which is due to Debye, is as follows, for instance, refer to Von Hippel, 1954, pp. 38 [1]:

According to the assumption of dominating friction, water molecules are considered to rotate under the torque γ of the electric field with angular velocity $\partial\theta/\partial t$ proportional to this torque, or

$$\gamma = \xi \frac{\partial\theta}{\partial t}, \quad (10)$$

where ξ is a constant of proportionality, termed as the friction factor. ξ depends on the shape of the molecule and on the type of interaction it encounters. If the molecule is visualized as a sphere of radius 'a' rotating in water of viscosity η , then according to Stoke's law, classical hydrodynamics leads to the value,

$$\xi = 8\pi\eta a^3. \quad (11)$$

When water is subjected to an electric field, then the dipoles experience a torque and tend to align in the direction of the field. This produces a polarization termed as the 'orientation polarization' as mentioned before. When the field is switched on, a certain time is required for the dipoles to orient in such a way that the polarization increases to $[1-(1/\exp)]$ of its final value in the presence of the field (where 'exp' is the base of natural logarithm). This time is the dipole relaxation time τ_d (of Debye, say) for water molecules. Debye has calculated this time statistically by deriving the space orientation under the counteracting influences of the Brownian motion and of a time dependent electric field and has found,

$$\tau_d = \frac{\xi}{2kT}, \quad (12)$$

where k is Boltzmann constant and T is temperature of water.

Combining eqns. (11) and (12), Debye has obtained for the spherical molecule of water, the relaxation time,

$$\tau_d = \frac{4\pi a^3 \eta}{kT}. \quad (13)$$

Now water at temperature ($T = 293^{\circ}\text{K}$), has the coefficient of viscosity $\eta = 1 \times 10^{-3} \text{ Nw-sc/m}^2$ (Clark 1988, pp. 62) [10]. If the radius 'a' of water molecule is taken as 2 A.U. or $2 \times 10^{-10} \text{ m}$, then eqn. (13) gives $\tau_d = 0.2485(4) \times 10^{-10} \text{ sc}$. Thus the frequency f at which $\omega\tau_d = (2\pi f)\tau_d = 1$ (refer also to Fig. 1) is given by this value of $f = 6.403(6) \times 10^9 \text{ Hz}$. This

value of f corresponds to a free space wavelength of $4.681(3) \text{ cm}$. Thus, the relaxation time τ_d of water molecules corresponds to the free space wavelength of $4.681(3) \text{ cm}$, in the relaxation spectrum of water at temperature $T = 293^{\circ}\text{K}$. But experimentally the relaxation time for water molecules at temperature $T = 293^{\circ}\text{K}$ is located near the free space wavelength of 1 cm in the relaxation spectrum as mentioned by Von Hippel (1954, pp. 38, fig. 4.2) [1]. Although there is a difference in the theoretical and experimental values of the free space wavelengths at which the relaxation time is located in the relaxation spectrum of water at temperature $T = 293^{\circ}\text{K}$, still the essence of the model of Debye is that even if it is approximate, this approach postulates that the orientation of water molecules leads to a simple relaxation spectrum in r.f. region of electromagnetic waves, similar to that as shown in Fig. 1.

In the present paper an analysis of dipole relaxation time of the molecule in water at temperature $T = 293^{\circ}\text{K}$ is carried out as an extension of the theory of coupled mass- vibrations of ions or atoms in noble metals or intrinsic germanium and silicon as considered previously by Nandedkar (2015) [11] and Nandedkar (2015) [12].

Here the water medium is considered as an intermediate one to a solid-state and a gaseous-state. The water molecule undergoes coupled mass-vibrations at the temperature $T (=293^{\circ}\text{K})$ on one hand and on other hand it possesses an average thermal velocity $v_w = (8kT/\pi M_w)^{1/2}$ as given by the kinetic theory of gases. Here k is Boltzmann constant and M_w is the mass of water molecule. Such a system of the water molecules is in thermal equilibrium at the temperature $T (=293^{\circ}\text{K})$, to which the r.f. electric field is applied [- where the dielectric absorption losses due to ϵ_r'' in presence of the r.f. electric field, causes an increase in temperature of the water accounting for the heat losses. And the temperature $T (=293^{\circ}\text{K})$ in the present analysis denotes an average temperature attained by the water in presence of these heat losses relative to surroundings in equilibrium conditions]. The thermal equilibrium is brought into the picture by molecule-molecule collisions in the water which are described by gas kinetics, where a molecule has got the coupled mass-vibrational mode and also simultaneously has an average thermal velocity. In other words, this is a quasi-stationary: quasi-moving system of the molecules of water undergoing coupled mass-vibrations and having the average thermal molecular velocity at temperature $T (=293^{\circ}\text{K})$ of the water under consideration, resulting in molecule-molecule collisions bringing about the thermal equilibrium.

The effective collision cross-section of molecule-molecule collisions is considered as proportional to the overall average of the resultant mean square amplitudes of the water molecule

undergoing coupled mass-vibrations at the temperature T ($=293^{\circ}\text{K}$). It is assumed that the water molecules are elastically bound with respect to each other so far as the coupled mass-vibrational modes are concerned. And further, the coupled mass-vibrational modes of the molecules are associated with the elastic waves in transverse mode of Debye type in the water. Only average values are treated in the calculations of transverse elastic wave velocity needed for the effective collision cross-section of the molecule-molecule or molecular collisions.

Then knowing the molecular collision frequency, the relaxation time of the molecular collisions is obtained considering it to be the reciprocal of the collision frequency, which has dimension of time.

This relaxation time is considered the same as the dipole relaxation time of the dipoles associated with the water molecules and interacting with the r.f. electric field.

The method of analysis of this research-paper consists of following sections for this article:

2. Mass-Vibrations of the Water Molecule
3. Molecular Collision Frequency and Dipole Relaxation Time
4. Numerical Analysis and
5. Conclusions

followed by Appendix which gives List of Symbols used.

2. Mass-Vibrations of the Water Molecule

Here analysis of mass-vibrations of the water molecules is carried out assuming that they are quasi-stationary.

Now consider one of the water molecules. The Molecule of the water is assumed to undergo thermal mass-vibrations at temperature T ($=293^{\circ}\text{K}$) of it. If M_w be the mass of the molecule having f' as the frequency of the mass-vibrations, then its equation of motion, say along x-axis can be written as follows:

$$M_w \frac{\partial^2 x}{\partial t^2} + 4\pi^2 f'^2 M_w x = 0, \quad (14)$$

where x is the displacement of the molecule from its (quasi-stationary) position of equilibrium at instantaneous time t when it has an acceleration of $\partial^2 x / \partial t^2$. Eqn. (14) is an equation of Simple Harmonic Motion.

The average potential energy V_w of the molecule over a cycle of its vibrations is given by,

$$V_w = 2\pi^2 f'^2 M_w x_{ow}^2, \quad (15)$$

where x_{ow} is the r.m.s. value of the amplitude of the

mass-vibrations of the molecule along x- axis.

If the weight factor to have V_w at temperature T be defined by the Boltzmann factor, viz.,

$$P(V_w) = \exp\left(-\frac{V_w}{kT}\right), \quad (16)$$

where k is Boltzmann constant, then the average value of x_{ow}^2 i.e. \bar{x}_{ow}^2 over various values of x_{ow}^2 for the molecular mass-vibrator with frequency f' can be obtained by averaging all values of x_{ow}^2 with the weight factor given by eqn.(16). Thus.

$$\bar{x}_{ow}^2 = \frac{\int_0^{\infty} x_{ow}^2 P(V_w) \partial x_{ow}}{\int_0^{\infty} P(V_w) \partial x_{ow}}. \quad (17)$$

Using eqns. (15) and (16), eqn. (17) gives on solving the integral that,

$$\bar{x}_{ow}^2 = \frac{kT}{(2\pi f')^2 M_w}. \quad (18)$$

Similarly for the directions of vibrations of the molecule along y- and z- axes, it can be shown that,

$$\bar{y}_{ow}^2 = \frac{kT}{(2\pi f')^2 M_w}, \quad (19)$$

and

$$\bar{z}_{ow}^2 = \frac{kT}{(2\pi f')^2 M_w}, \quad (20)$$

respectively. Whence the resultant average of mean square amplitudes of the molecular mass-vibrations averaged with the Boltzmann factor i.e. \bar{R}_{ow}^2 is given by,

$$\bar{R}_{ow}^2 = \bar{x}_{ow}^2 + \bar{y}_{ow}^2 + \bar{z}_{ow}^2 = \frac{3kT}{(2\pi f')^2 M_w}. \quad (21)$$

The quasi-stationary molecules of the water are considered to have elastic bindings with respect to each other. These molecules are assumed to undergo mass-vibrations at temperature T ($=293^{\circ}\text{K}$) of the water in the presence of transverse elastic (acoustic) waves existing in the water. Frequency of the mass-vibrations of the molecules is considered to be the same as that of the transverse elastic wave (acoustic wave) of Debye type.

Considering the water as continuous medium, so far as the propagation of transverse elastic waves are concerned, the number of transverse elastic wave modes per unit volume of the water denoted by $Z_w(f') \partial f'$ in frequency interval $\partial f'$ between f' and $f' + \partial f'$, is given by

$$Z_w(f') \partial f' = 4\pi f'^2 \left(\frac{z}{v_l^3}\right) \partial f', \quad (22)$$

using a similar approach as mentioned in the case of transverse elastic wave modes in noble metals/intrinsic Ge & Si in a previous paper by Nandedkar (2015) [11]/Nandedkar (2015)

[12]. Here in the water longitudinal elastic waves are considered not to exist. Here v_t denotes the velocity of transverse elastic wave in water. This analysis assumes that the linear dimensions of the water are extremely large as compared to the inter-molecular distance(s). The water is of macroscopic dimensions and of conventional sizes.

If N_w is the density of molecules in the water, then there would be $3N_w$ modes of elastic waves per unit volume because there are $3N_w$ degrees of freedom per unit volume for mass-vibrations of the molecules along three mutually perpendicular axes. This limits the maximum frequency of the wave. If minimum frequency be taken zero for all practical purposes and maximum be denoted by Debye frequency f_D' of cut-off, then,

$$\int_0^{f_D'} Z_w(f') \partial f' = 3N_w, \quad (23)$$

meaning thereby coupled mass-vibrational modes of the molecules take place in the presence of elastic wave modes in the water. And further each of the molecules has a band of frequency ranging 0 to f_D' for all practical purposes, when the linear dimensions of the water are extremely large as compared to the inter molecular distance(s).

Further using eqn. (22) in eqn. (23), eqn. (23) gives

$$\int_0^{f_D'} 4\pi f'^2 \left(\frac{2}{v_t^3}\right) \partial f' = 3N_w. \quad (24)$$

Solution of eqn. (24) gives,

$$f_D' = \left(\frac{9N_w v_t^3}{8\pi}\right)^{1/3}, \quad (25)$$

where it is assumed that the elastic wave velocity is independent of frequency.

Coming to eqn. (22), $Z_w(f')$ gives the weight-factor to have the elastic waves of molecular mass vibrations at frequency f' . Further the average of \bar{R}_{ow}^2 with respect to the weight-factor $Z_w(f')$ is given by,

$$\langle \bar{R}_{ow}^2 \rangle = \frac{\int_0^{f_D'} \bar{R}_{ow}^2 Z_w(f') \partial f'}{\int_0^{f_D'} Z_w(f') \partial f'}. \quad (26)$$

Using eqns. (21), ((22) and (23), eqn. (26) gives,

$$\langle \bar{R}_{ow}^2 \rangle = \frac{\int_0^{f_D'} \left[\frac{3kT}{(2\pi f')^2 M_w} \right] 4\pi f'^2 \left(\frac{2}{v_t^3}\right) \partial f'}{3N_w}, \quad (27)$$

which on simplification gives that,

$$\langle \bar{R}_{ow}^2 \rangle = \left(\frac{kT}{\pi\rho}\right) \left(\frac{2}{v_t^3}\right) f_D', \quad (28)$$

where,

$$\rho = M_w N_w, \quad (29)$$

gives the density of the water.

Using eqn. (25), eqn. (28) gives that,

$$\langle \bar{R}_{ow}^2 \rangle = \left[\left(\frac{2k}{\pi\rho}\right) \left(\frac{9N_w}{8\pi}\right)^{1/3} \frac{1}{v_t^3} \right] T. \quad (30)$$

Equation (30) gives the overall average of the resultant mean square amplitudes of the mass-vibrations of the molecule in the water undergoing coupled mass-vibrations at temperature T ($= 293$ °K) of it, where the molecule is considered in the quasi-stationary state of this analysis.

3. Molecular Collision Frequency and Dipole Relaxation Time

If N_w be the molecule density in the water, Q_w be the effective collision cross-section for the molecular collisions and v_w be the average thermal molecular velocity considering one of the molecules in quasi-moving state at temperature T ($=293$ °K) given by kinetic theory of gases, viz.,

$$v_w = \left(\frac{8kT}{\pi M_w}\right)^{1/2}, \quad (31)$$

then the molecule-molecule or the molecular collision frequency v_{ow} using gas-kinetics is given by,

$$v_{ow} = N_w Q_w v_w \quad (32)$$

Here the effective collision cross-section is considered as proportional to $\langle \bar{R}_{ow}^2 \rangle$ i.e. to the overall average of the resultant mean square amplitudes of the mass-vibrations of the molecule in the water undergoing coupled mass-vibrations at temperature T ($= 293$ °K) of it as given by eqn. (30), considering-quasi stationary state of the rest of the molecules other than the one in quasi-moving state with the average thermal velocity given by eqn. (31), where $N_w \gg 1$. And Q_w for the spherical water molecule in the present analysis is considered here as given by,

$$Q_w = \pi \langle \bar{R}_{ow}^2 \rangle. \quad (33)$$

Eqn. (33), using eqn. (30) gives that

$$Q_w = \pi \left[\left(\frac{2k}{\pi\rho}\right) \left(\frac{9N_w}{8\pi}\right)^{1/3} \frac{1}{v_t^3} \right] T. \quad (34)$$

Further using eqns. (31) and (34) in eqn. (32), eqn. (32) gives that

$$v_{ow} = N_w \pi \left[\left(\frac{2k}{\pi\rho}\right) \left(\frac{9N_w}{8\pi}\right)^{1/3} \left(\frac{1}{v_t^3}\right) \left(\frac{8k}{\pi M_w}\right)^{1/2} \right] T^{3/2}, \quad (35)$$

where v_{ow} gives the collision frequency of the water molecules.

Now $1/v_{ow}$ has the dimensions of time. And $1/v_{ow}$ is denoted by τ_{ow} . The value of τ_{ow} is given by,

$$\tau_{ow} = \frac{1}{v_{ow}} = \frac{\left[\left(\frac{2k}{\pi\rho} \right) \left(\frac{9N_w}{8\pi} \right)^{1/3} \left(\frac{1}{v_t^2} \right) \left(\frac{8k}{\pi M_w} \right)^{1/2} \right]^{-1}}{N_w \pi} T^{-3/2}, \quad (36)$$

using eqn. (35). In the present analysis it is considered that τ_{ow} of eqn. (36) as given by gas- kinetics is the relaxation time of molecule-molecule collisions/molecular collisions or it is relaxation time between collisions of the (water) molecules.

Now come to eqn. (30). Here $\langle \bar{R}_{ow}^2 \rangle$ is treated as the overall average of the resultant mean square amplitudes of the mass-vibrations of the molecule (of the dipole) in the water undergoing coupled mass-vibrations at temperature T ($=293$ °K) of it. Further, eqn. (31) gives the average thermal velocity of the molecule (of the dipole) and eqn. (34) gives the effective collision cross-section of the molecule (of the dipole) collisions of the water molecules, respectively. Eqn. (36) represents the dipole relaxation time of the collision process having the collision frequency v_{ow} of eqn. (35) at temperature T ($=293$ °K) for the water molecules.

When the water is subjected to the r.f. electric field, then the dipoles experience a torque and tend to align in the direction of the field. This produces the orientation polarization, and would give rise to a relaxation spectrum similar to that given in Fig. 1 as mentioned in Secn.1. Here T ($=293$ °K) gives the average temperature attained by the water in the presence of dielectric absorption losses due to ϵ_r'' relative to surroundings in equilibrium conditions, in the presence of r.f. electric field which is applied to the system of dipoles of water molecules.

In short, the orientation polarization of water molecules in the presence of r.f. electric field(s) would lead to a relaxation spectrum similar to that as show in Fig. 1, which is characterized by a molecular (dipolar) relaxation time of τ_{ow} as given by eqn.(36) at the temperature T ($=293$ °K) of the water under consideration.

4. Numerical Analysis

If ρ be the density and M_m be the molecular weight of water, then the density of molecules (or dipoles) in the water, is given by

$$N_w = \frac{N_a \rho}{M_m}, \quad (37)$$

where N_a is Avogadro's number.

Further if m_u is 1-unified mass unit, then the mass of a water molecule M_w is given by

$$M_w = m_u M_m. \quad (38)$$

The transverse elastic wave velocity v_t in the water can be shown to be given by {a similar approach as adopted in case of the noble metals/intrinsic Ge & Si by Nandedkar (2015) [11]/(2015) [12]},

$$v_t = \left(\frac{\eta'}{\rho} \right)^{1/2}, \quad (39)$$

where η' is (bulk) modulus of rigidity for water.

Table 1 gives the values of molecular weight M_m of water, density ρ and (bulk) modulus of rigidity η' for water from Clark (1988, pp.57-58, 62) [10]. The values of ρ and η' are at $T=293$ °K. T denotes temperature of the water. Calculated values of N_w, v_t and M_w are also given in Table 1.

Table 1. Physical constants of Water at $T = 293$ °K.

M_m	ρ	η'	N_w	v_t	M_w	
			10^{-9}	$\times 10^{-28}$	$\times 10^{-3}$	$\times 10^{26}$
(kgm-mol)	(kgm/m ³)	(Nw/m ²)	(m ⁻³)	(m/sc)	(kgm)	
18.01(6)	998	2.05	3.336(5)	1.433(2)	2.991(4)	

The values of overall average of the resultant mean square amplitudes of the mass vibrations of the water molecule $\langle \bar{R}_{ow}^2 \rangle$, the effective collision cross section Q_w , the average thermal velocity v_w , the collision frequency v_{ow} and the relaxation time τ_{ow} as given by eqns. (30), (33), (31), (32) and (36) respectively, are calculated using Table 1. These values refer to the water molecule or the dipole associated with the molecule. Here the temperature T of the water is 293 °K. The calculated results are given in Table 2.

Table 2. Various Parameters Associated with the Molecular (Dipole) Relaxation Time for the water at $T = 293$ °K.

$\langle \bar{R}_{ow}^2 \rangle$	Q_w	v_w	v_{ow}	τ_{ow}
$\times 10^{21}$	$\times 10^{21}$	$\times 10^{-2}$	$\times 10^{-11}$	$\times 10^{12}$
(m ²)	(m ²)	(m/sc)	(sc ⁻¹)	(sc)
2.871(7)	9.021(7)	5.867(9)	1.766(3)	5.661(6)

Thus here the effective collision cross section Q_w is $9.021(7) \times 10^{-21}$ m², and the collision frequency v_{ow} is $1.766(3) \times 10^{11}$ sc⁻¹, where sc stands for second. This gives the molecular or dipole relaxation time τ_{ow} of $5.661(6) \times 10^{-12}$ sc for the water at temperature $T = 293$ °K.

5. Conclusions

The frequency f at which angular frequency w of the r.f. field satisfies the condition $w\tau_{ow} = (2\pi f)\tau_{ow} = 1$ (similar to that as shown in Fig. 1), gives the value of $f = 2.811(1) \times 10^{10}$ Hz. This corresponds to the free space wavelength of 1.066(4) cm, at the temperature $T=293$ °K for the water [- here the dielectric absorption losses due to ϵ_r'' in presence of the r.f. electric field, causes an increase in temperature of the water accounting for the heat losses. And the temperature T ($=293$ °K) in the present analysis denotes an average

temperature in the presence of these heat losses relative to surroundings in equilibrium conditions].

Further, experimentally the relaxation time of water at temperature T of 293°K corresponds to a free space wavelength located near 1 cm in the relaxation spectrum of water, as mentioned by Von Hippel ([1954, pp.38, fig.4.2 [1]), whereas present analysis also detects that the relaxation time of water at temperature T of 293°K corresponds to a free space wavelength of 1.066(4) cm, that is, located near 1 cm in the relaxation spectrum of water. So present analysis fairly well predicts that the relaxation time of water at temperature T of 293°K corresponds to a free space wavelength of 1.066(4) cm, that is, located near 1 cm in the relaxation spectrum of water.

Now refer to Secn. 1, Fig. 1 of the present paper, as well as Von Hippel (1954, pp.38, fig. 4.2 [1]) - (which has break for free space r.f. wavelengths shorter than about 8 mm)], which is considered to hold good in the r.f. region of spectrum of electromagnetic waves up to a minimum of about 8 mm of the free space r.f. wavelengths for water of this treatment. In the present paper, it is considered that for the free space r.f. wavelengths shorter than about 8 mm, the thermal energy of the dipole of water at temperature $T=293^{\circ}\text{K}$ is insufficient to align the dipole (of molecule) of water because of the torque experienced by it (in presence of r.f. electric field) against the force due to molecular collision (- here also refer to Kittel, 1960, pp.176 [13], for corresponding views on the water model of Debye).

Thus the present model given in this paper determines fairly well the molecular (dipole) relaxation time for water at temperature of 293°K , which is experimentally located near the free space wavelength of 1 cm in the relaxation spectrum of water.

The analysis of this paper assumes that for the water under consideration, it is possible to define the dipole relaxation time for the water molecules by eqn. (36), which is based on assumption of eqn. (14).

Appendix

List of Symbols Used

N_w = water molecules per unit volume

$^{\circ}\text{K}$ = degree Kelvin

μ = magnitude of permanent dipole moment associated with water molecule

τ_o = dipole relaxation time of water molecule (general)

$P(t)$ = polarization at time t

$P(\infty)$ = steady state final polarization

\exp = base of natural logarithm

$i = \sqrt{-1}$

ϵ_r = relative static permittivity of water with respect to free space

ϵ_o = permittivity of free space

E = Instantaneous value of r.f. electric field at time t

E_o = peak value of the r.f. electric field

f = frequency of r.f. electric field

w = angular frequency of r.f. field = $2\pi f$

ϵ_r^* = relative complex dielectric constant of water with respect to free space

ϵ_r' = relative r.f. permittivity of the water with respect to free space

ϵ_r'' = relative r.f. loss factor of the water with respect to free space

γ = torque of the electric field with reference Debye model

$\partial\theta/\partial t$ = molecular angular velocity with reference Debye model

ξ = a constant of friction factor with reference Debye model

η = coefficient of viscosity of water

a = radius of water molecule with reference Debye model

τ_d = dipole relaxation time of water molecule with reference Debye model

T = temperature

k = Boltzmann constant

M_w = mass of water molecule

f' = frequency of the mass-vibrations of water molecule

V_w = average potential energy of the water molecule over a cycle of its vibrations

x = displacement of the molecule from its (quasi-stationary) position of equilibrium at instantaneous time t when it has an acceleration of $\partial^2x/\partial t^2$

x_{ow} = r.m.s. value of the amplitude of the mass-vibrations of the molecule along x- axis

$P(V_w)$ = weight factor to have V_w at temperature T defined by the Boltzmann factor

\bar{x}_{ow}^2 = average value of x_{ow}^2 over various values of x_{ow}^2 along x-axis

\bar{y}_{ow}^2 = average value of y_{ow}^2 over various values of y_{ow}^2 along y-axis

\bar{z}_{ow}^2 = average value of z_{ow}^2 over various values of z_{ow}^2 along z-axis

\bar{R}_{ow}^2 = resultant average of mean square amplitudes of the molecular mass-vibrations averaged with the Boltzmann factor considering 3-axes of co-ordinates

$Z_w(f')$ = number of transverse elastic (acoustic) wave modes per unit volume per unit frequency interval in the water

v_t = velocity of transverse elastic (acoustic) wave in water

f'_D = Debye frequency of cut-off

ρ = density of water

$\langle \bar{R}_{ow}^2 \rangle$ = average of \bar{R}_{ow}^2 with respect to the weight-factor $Z_w(f')$

Q_w = effective collision cross-section for the molecular collisions

v_w = average thermal molecular velocity of water

ν_{ow} = molecule-molecule or molecular collision frequency in water

τ_{ow} = dipole relaxation time for water molecules = $1/\nu_{ow}$ (of this paper)

M_m = molecular weight of water

N_a = Avogadro's number

m_u = 1-unified mass unit

η' = (bulk) modulus of rigidity for water

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