

## Molecular Dynamics Study of Microwave Heating of Water and Aqueous Solutions

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We show by molecular dynamics simulations that liquid water is heated by applied microwaves through excitation of rotational alignment and subsequent relaxation of electric dipoles. Small addition of salt to water increases the heating rate. Crystal ice is much less heated and hydrogen-bonded molecular network remains intact under the microwaves.

マイクロ波による水の加熱過程を分子動力学法により研究し、加熱が分子回転の励起と衝突緩和によること、塩添加した水溶液の加熱率が上昇すること、結晶化した氷はあまり加熱されないことを示した。

### 1. Introduction

Electromagnetic waves can heat solid, liquid and gaseous matters including gels/polymers, engineering materials, laboratory plasmas and even living cells. A microwave ovens used in daily food processing is one of such examples where heating is believed to occur through the rotational absorption of applied electromagnetic waves by water molecules. The purpose of this study is to investigate the heating process of water and salt solutions by applied microwaves in terms of the classical molecular dynamics simulations.

We use the microwaves of 10GHz (to speed up the simulations) whose wavelength is 3cm. Since the molecular scale is much less than this length, and since all the involved velocities are much less than the speed of light ( $v/c \ll 1$ ), we can safely assume that the waves are spatially uniform, time varying electric field of the form  $E(t) = E_0 \cos(\omega t)$ . We put approximately 2700 water molecules and also small number of salt ions in a cubic box of 45 Angstroms in each side. Water molecules are represented by the rotating rigid body known as the SPC water model [1] which consists of three point charges 0.42e, 0.42e, -0.84e located at two hydrogen and one oxygen sites, respectively. These molecules move under the Coulombic and Lennard-Jones forces which are exerted by surrounding molecules [2].

Three types of runs are performed, namely, (i) pure water at 300K, (ii) ice of the Ic form, and (iii) salty water with 1mol% NaCl (roughly 3wt% or 0.5M) at 300K. The initial configuration is prepared by randomizing the

hydrogen bonds of the ice crystal [3]. These molecules are set to a given temperature during the equilibration phase, after which the microwave electric field is switched on.

Due to thermal fluctuations, we have to use an enhanced electric field in the simulations which is typically  $E \sim 1 \times 10^6 \text{ V/cm}$ . On the other hand, we note that this is not a large electric field viewed from water molecules since the dipole energy  $E_d \sim 2.4 \times 10^{-3} \text{ eV}$  is still less than thermal energy  $kT \sim 2.6 \times 10^{-2} \text{ eV}$  at room temperature, and by orders of magnitude less than the hydrogen bond energy  $5 \text{ eV/bond}$ .

### 2. Results

Figure 1 shows the time history of (a) the applied microwave field, (b) the potential energy (Coulombic + Lennard-Jones), and (c) the total energy of the system. During the

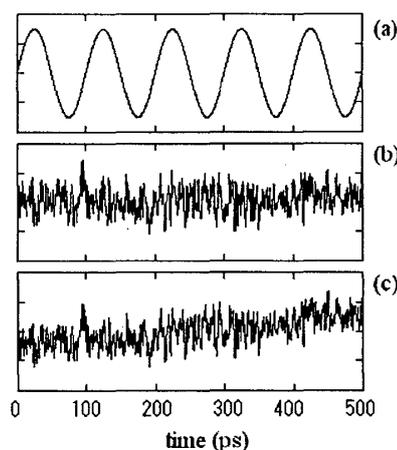


Fig.1: The time history of (a) the applied microwave field, (b) potential energy and (c) total energy of the system for water of 300K and 2700 molecules.

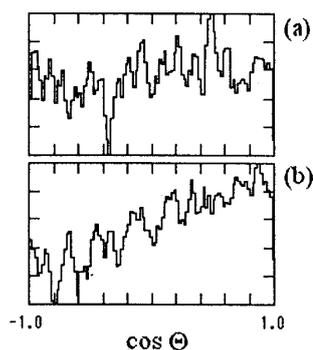


Fig.2. The distribution of water dipoles (logarithmic scale) in terms of the angles  $\Theta$  with the x-axis for water of 300K. The microwave electric field is null in (a) and points to the x direction in (b).

application of the microwave field, the potential energy is almost conserved, while the total energy of the system increases after the initial transient phase  $t > 180\text{ps}$ . This increase is attributed to that in the translational energy resulting from rotation excitation and relaxation of water molecules. Distributions of the water dipoles in terms of the directional cosine of their angles with the x-axis  $\cos\Theta$  are shown in Fig.2 for (a)  $E=0$  and (b)  $E=E_0x$ . For room temperature water, the molecular dipoles distribute randomly. However, with the finite microwave field the dipoles align along the electric field direction and follow at each instant the statistical (Boltzmann) distribution  $\exp(-E d \cos\Theta / kT)$  [ $d$  is the dipole moment of  $\text{H}_2\text{O}$ ]. The heating rate of water appears to scale as  $dT/dt \sim E^{1.1}$  with the microwave field and decreases with the temperature.

By contrast, the water in ice state is hardly heated by microwave. This is reflected in the almost invariant distributions of ice dipoles of Fig.3 for the same microwave field as that used in Fig.2. The bird's-eye view snapshots

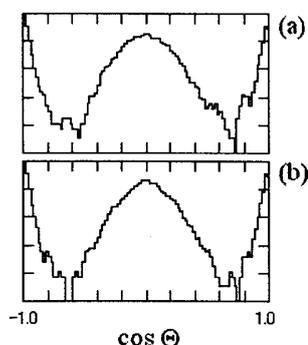


Fig.3 The distribution of ice dipoles for the crystal ice of 230K. The microwave fields are the same as those in Fig.2.

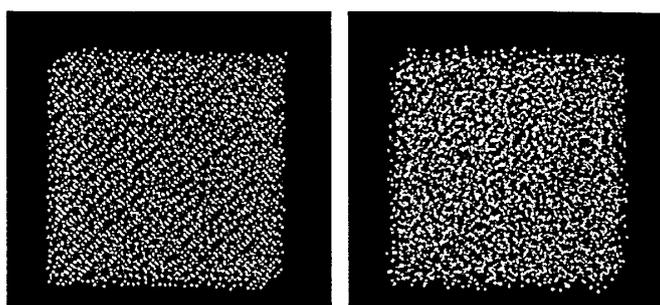


Fig.4 The bird's-eye view of water molecules at the beginning (left, ice crystal) and at 150ps after application of the microwave (right) for 300K water with 2700 molecules.

of water molecules for room temperature in Fig.4 reveal this situation. All the simulations start from the crystal ice of 6-membered ring network (Fig.4, left), which melts and becomes randomized for the room temperature case (Fig.4, right). For the ice case, the initial structure is nearly preserved even after the application of strong microwaves.

When salt of 1mol% NaCl is added to liquid water, the heating rate increases by 50%. This increase may be attributed to the breakage of the water network by finite size salt ions. The diameter of  $\text{Na}^+$  is 2.6Å and is 4.4Å for  $\text{Cl}^-$ . These diameters are comparable to the cell size of the water network, and they are forming hydrated ion clusters  $\text{Na}(\text{H}_2\text{O})_n$  typically with  $n=5\sim 6$ .

### 3. Conclusion

Heating of water by microwaves was shown to occur through the excitation of electric dipole rotation and its relaxation. Crystal ice was much less heated than liquid water because of rigid hydrogen-bonded molecular network.

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### References

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