Heating of Water and Ionic Solutions by Applied Microwaves: Molecular Dynamics Study

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Electromagnetic waves heat solid, liquid and gaseous matters such as engineering materials, laboratory plasmas and biological matters including living cells. A microwave ovens used in daily food processing is one of such examples. The purpose of this study is to investigate the heating process of water and salt solutions by applied microwaves in terms of classical molecular dynamics simulation. We have shown that water in liquid state is heated by applied microwave through excitation of rotational motion of electrical dipoles. Salt water is heated a few times better than pure water because of the Joule heating of salt ions, but crystal ice is hardly heated due to hydrogen-bonded molecular network.

We use the microwaves of 10GHz 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 ($v/c<<1$), we can safely assume that the waves are represented by spatially uniform, time varying electric field of the form $E(t)= E_0\cos(\omega t)$. Water molecules are modeled by the rotating rigid body known as the SPC water model [1]. We adopt crystal ice for the initial conditions with randomized O-H directions [2]. These molecules move under the Coulomb and Lennard-Jones forces which are exerted by surrounding molecules [3].

The total energy of the system increases when the AC electric field is applied. The observed heating is attributed to the increase in the rotational energy resulting from excitation of rotational motion of electrical dipoles and subsequent relaxation to translational energy. Distributions of the water dipoles in terms of the directional cosine of their angles with the electric field $\cos\Theta$ are shown in Fig.1. 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 $\exp(-Ed\cos\Theta /kT)$ [d is the dipole moment of H_2O]. Dilute salt water with 1mol% Na^+Cl^- is twice more heated than pure water, in which we observe sloshing motion of salt ions in response to the applied AC field. By contrast, the water in ice state is hardly heated by microwave. This is due to the formation of rigid hydrogen-bonded network in crystal ice. The bird's-eye view of H_2O molecules for the ice state in Fig.2 reveals this situation.

References: [1] H.Berendsen, J.Grigera, T.Straatsma, J.Phys. Chem. **91**, 6269 (1987).
[2] Initial configuration is due to courtesy of Dr. M.Matsumoto.
[3] Y.Rabin and M.Tanaka, Phys.Rev.Lett., **94**, 148103 (2005)

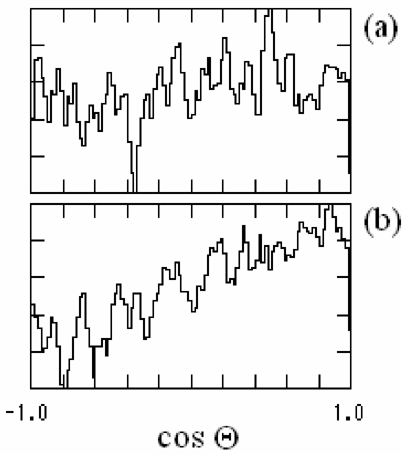

Fig.1. The angular distribution of water dipoles (logarithmic scale) in terms of the angles Θ with the AC electric field for water of 300K. The microwave electric field is null in (a) and is present in (b).

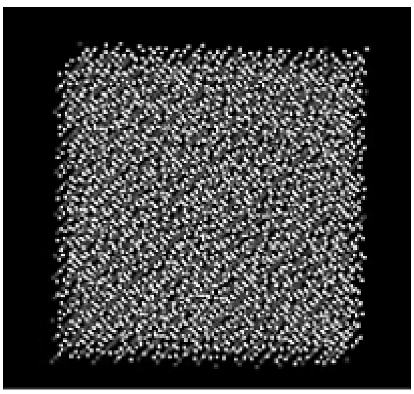

Fig.2 Bird's-eye view of 2700 H_2O molecules in ice state.