

§6. Microwave Heating of Salty Water and Ice: Heating Occurs, but Mechanisms are Different !

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Selective and efficient heating of materials is realized by microwave application because of local absorption of the wave energy in an atomistic level. The heating by microwaves (3-300GHz) ranges from heating of polarizable liquid including water [1] to sintering of solid materials such as metal oxide particles [2,3].

Previously, we showed three aspects of microwave heating of water and ice by molecular dynamics simulations [1]: (i) Liquid water is heated by rotational excitation of water molecules and irreversible energy transfer to kinetic (thermal) energy by collisions, (ii) pure ice is not heated because of strong hydrogen bonded crystal network, (iii) salty water is heated better than pure water due to Joule heating of salt (Na and Cl) ions. The last aspect was verified by directly measuring the ratio of the Joule heating rate to conventional dipole-rotational heating rate for 1mol% salty water:

$$|\mathbf{E} \cdot \mathbf{J}| / |\mathbf{E} \cdot d\mathbf{P} / dt| \approx 2$$

where \mathbf{E} is the microwave electric field and \mathbf{P} is the dipole moment of water molecules. This accounted for the experimentally known heating rate of such salty water, which is roughly three times that of pure water at room temperature (300K).

In the above work, pure ice was shown not to be heated by microwaves. A question still remains whether salt-added ice can be heated by applied microwaves. This is relevant to daily applications of melting frozen food in microwave ovens. Recently, we have found that salty ice is heated unlike pure ice, and it is due to “defects” of hydrogen-bonded network made by large Cl ions.

Our molecular dynamics simulation treats a charged N-body system with the Coulomb and Lennard-Jones forces [1]

$$m_i \frac{d\mathbf{v}_i}{dt} = \sum_j \frac{q_i q_j}{|\mathbf{r}_i - \mathbf{r}_j|} + 48\epsilon_{ij} \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^6 \right],$$

$$\frac{d\mathbf{r}_i}{dt} = \mathbf{v}_i$$

Here, \mathbf{r}_i and \mathbf{v}_i are the position and velocity of i-th particle, respectively, m_i and q_i are its mass and charge, respectively, σ is the sum of radii of i-th and j-th

particles, and ϵ_{ij} is the Lennard-Jones energy. For water molecules, the SPC/E explicit water model is adopted, in which H and O atoms are partially charged with +q and -2q, respectively, with $q=0.424e$, and σ is 3.17Å (Angstroms). It is stressed that $\sigma=2.6\text{Å}$ and 4.4Å for Na^+ and Cl^- ions, respectively so that large Cl^- ions do not fit in a cell of the water network, thus providing for defects.

Figure 2 shows the time history of electric dipole moment of the whole system for 1mol% salt-added ice (top) and pure water (bottom). Solid and gray lines show the dipole moment and applied microwave electric field, respectively. Unlike pure ice, the dipoles of water molecules can rotate in salty ice. Thus, salty ice is heated by microwaves and finally melts around 8-th period in Figure 2. The heating rate is comparable to that of pure water, but the measured ratio of the Joule and dipole heating rates $|\mathbf{E} \cdot \mathbf{J}| / |\mathbf{E} \cdot d\mathbf{P} / dt|$ is much less than unity for salty ice. Therefore, this heating is due to rotational excitation of electric dipoles of molecules in “ice” because of weakening of the network, which should be caused by inclusion of large Cl ions.

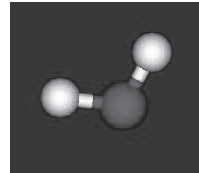


Fig.1 Explicit rigid water model SPC/E used in the present study. Oxygen (red) and hydrogen (gray)

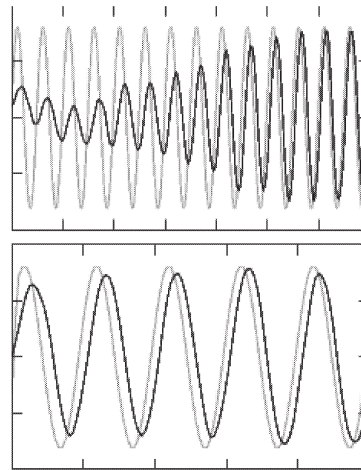


Fig.2 Time history of the amplitude of dipoles (solid) and microwave electric field (gray) for salty ice and pure water in top and bottom panels, respectively.

Time (period)

References

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- [3] “Science and Technology of Microwave- Induced Non-Equilibrium Reaction Fields”, MEXT Grant-in-Aid for Specific Research Areas (FY2006-10). <http://phonon.nifs.ac.jp/>