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Investigate the microscopic properties and the non-thermal effect of the electrolyte solution under microwave irradiation

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ABSTRACT

Non-equilibrium molecular dynamics (NMD) simulations are performed to investigate the microscopic properties and the non-thermal effect of microwave irradiation on NaCl electrolyte solution at different temperatures using the SPC/E model. The electromagnetic wave propagates in the *z*-axis direction with a frequency of 2.45 GHz, and the intensity of the *E*/*H* field is 3.4×10^4 V/m. The results indicate that as the concentration of the electrolyte solution increased, the electrical conductivity gradually increased, but the hydrogen bonds number and the coordination number decreased. In addition, the change of conductivity decreases with the increase of temperature when electromagnetic field is applied.

1. Introduction

Electrolyte is a very important material for natural living system and industrial processes, and hence many chemists and physicists have extensively investigated its structure and properties [1–6]. Microwave heating is an important industrial process, and recently, there has been increased focus on the application of microwave radiation for synthesis of catalysts and so on [7–9]. Many studies have investigated the effects of electromagnetic radiation on electrolyte [10–14]. Research has shown that the properties of electrolyte can be change under the electromagnetic field, and some have even found the microwave non-thermal effects [15–17].

In this Letter we have studied the microscopic properties and non-thermal effects of microwave fields at 2.45 GHz and the root-mean-square (RMS) field strengths 3.4×10^4 V/m on electrolyte solution by using non-equilibrium molecular dynamics (NEMD). The objectives of this Letter were to ascertain the existence of non-thermal effects, which influences the conductivity.

2. Simulation details

2.1. Incorporation of E/M field

The introduction of an external electrical and magnetic fields into a molecular dynamics (MD) simulation requires a time-dependent forcing function in Newton's second law, to describe the forces exerted on the charge sites by the field. For the electrical and magnetic fields, *E* and *H*, the forces acting on each charge site are incorporated as follows [18]:

$$m_i\vec{a}_i = q_i\vec{E}(t) + q_i\vec{v}_i \times \mu\vec{H}(t) \tag{1}$$

where q_i is charge, μ is permeability [19], $\vec{E}$ and $\vec{H}$ are taken to be uniform and plane-polarized in the *z* direction. The electric field component $\vec{E}(t)$ and magnetic field component $\vec{H}(t)$ are taken respectively to act in *x* and *y* direction as:

$$\begin{aligned}\vec{E}(t) &= E_{\max}\cos(\omega t)(1\vec{i} + 0\vec{j} + 0\vec{k})\\ \vec{H}(t) &= H_{\max}\sin(\omega t)(0\vec{i} + 1\vec{j} + 0\vec{k})\end{aligned} \tag{2}$$

In Eq. (1), the force $q_i\vec{E}$ is directed in the *x* direction only, ipso facto. However, the force $q_i v_i \times \mu\vec{H}$ is directed in *x* and *z* directions as:

$$\begin{aligned}q_i\vec{v}_i \times \vec{B} &= \mu q_i(v_{i,x}\vec{i} + v_{j,y}\vec{j} + v_{k,z}\vec{k}) \times (0\vec{i} + H(t)\vec{j} + 0\vec{k})\\ &= \mu q_i H(t)(-v_{i,z}\vec{i} + 0\vec{j} + v_{i,x}\vec{k})\end{aligned} \tag{3}$$

2.2. Simulation details

The water molecules were characterized by the SPC/E model in all simulations [20]. All ions were represented by a point charge having a *Lennard–Jones* center on it. The potential parameters for ion–water and water–water interactions in this model were collected from the work of Lee [21].

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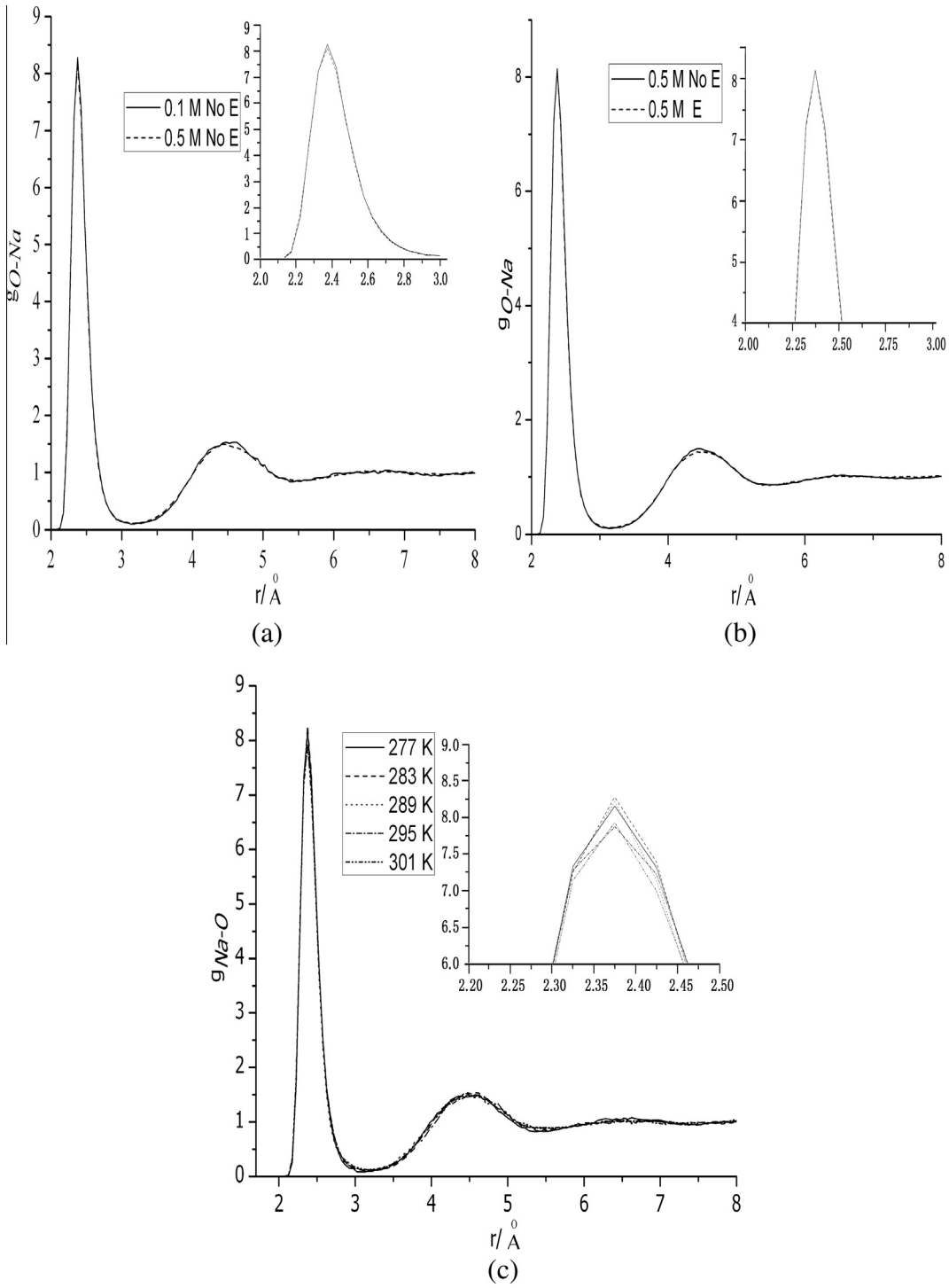

Figure 1. Radial distribution functions of Cation–O. (a) 0.1 and 0.5 M electrolyte solution without the electromagnetic field; (b) 0.5 M electrolyte solution with or without the electromagnetic field at 283 K; (c) 0.1 M electrolyte solution at different temperature and without the electromagnetic field.

The simulations involved a total of 4000 water molecules, contained within an isotropic simulation box, and considered two different NaCl solution concentrations, i.e., 0.1 and 0.5 M (molality), corresponding to 7 Na^+, 7 Cl^- and 35 Na^+, 35 Cl^-, respectively. The Nosé-Hoover [22,23] thermostat was used to maintain the equilibrium temperature at 277, 283, 289, 295 and 301 K, and periodic boundary conditions were imposed in all three dimensions. Accordingly, the Nosé-Hoover thermostat was used to study the non-thermal effects of the electromagnetic field on the electrolyte solution in our simulation. The trajectories of the atoms during the equilibration process were calculated using the Verlet velocity algorithm [24]. To ensure the pressure of the two systems were the same (1 bar), the NPT ensemble was carried out in the pre-equilibrium process. The *E*/*H* field was applied in the NVT ensemble to isolate the thermal effects, and hence the simulations were effectively non-equilibrium NVT (NNVT) ones. External *E*/*H* fields were applied to those models, all of the fields were of frequency $f = 2.45$ GHz, and the root-mean-square (RMS) electric field intensities were $E_{RMS} = 3.4 \times 10^4$ V/m [25], respectively.

During the MD simulation, a time step of 1 *fs* was used in all simulations; a period of 50 *ps* was allowed for equilibration (NPT ensemble). Following the equilibration process, an *E*/*M* field of