Title: Frequency-dependent electrical characteristics of DNA using molecular dynamics simulation

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Extended summary:

Researches on DNA have been widely carried out as promising materials for nano-electronics along with medicine development and disease test, from the aspects of experiments, simulations and theories. We have carried out molecular dynamics simulation coupled with the linear response theory, which based on time-correlation function of observable, to extract frequency-dependent electrical characteristics of DNA. The frequency dependent dielectric function $\varepsilon(\omega)$ and the conductivity $\sigma(\omega)$ for the MD simulation are simplified to[1]

$$\varepsilon(\omega) = 1 + 4\pi X_M(\omega)$$

$$\sigma(\omega) = X_J(\omega).$$

where the susceptibilities $X_M(\omega)$ and $X_J(\omega)$ are given by

$$X_M(\omega) = \frac{1}{3Vk_BT} + \left[< M(0)M(0) > + \iota\omega < M(0)M(t) >_\omega + < M(0)J(t) >_\omega \right]$$

$$X_J(\omega) = \frac{1}{3Vk_BT} + \left[\iota\omega < M(0)J(t) >_\omega + < J(0)J(t) >_\omega \right]$$

where M(t) and J(t) are, respectively, the total dipole moment of non-ionic atoms and the total electric current of ions at time t. These are given by

$\mathbf{M}(t)=\Sigma q_i \mathbf{x}_i$ (i: non-ionic atom)

$\mathbf{J}(t)=\Sigma q_i \mathbf{v}_i$ (i: ion atom)

where q_i is the charge of the ith atom. $<\ldots>_\omega$ denotes the Laplace transform

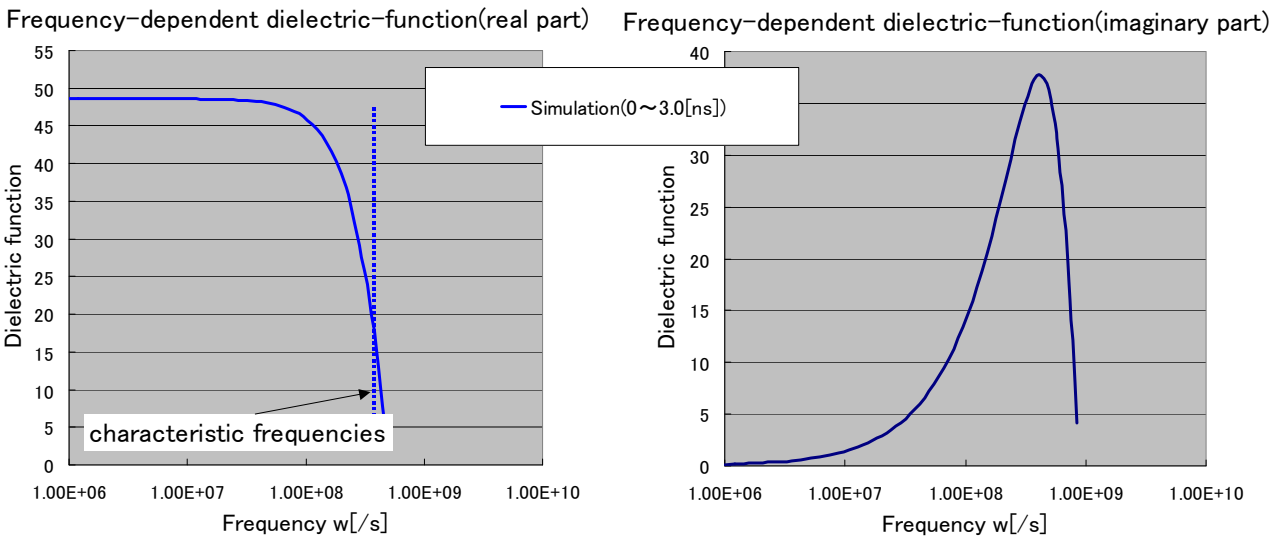
$<\ldots>_\omega = \int_0^\infty dt\, e^{i\omega t} <\ldots>$.

Figure 1(a) shows the frequency-dependent permittivity, which is the real part of the dielectric function, calculated from MD simulation results, and fig. 1(b) shows the imaginary part of the dielectric function. The MD simulation has been carrying out using the conditions listed on table 1.

We observe a dielectric relaxation around 50MHz in a case of 8bp-dsDNA, which corresponds to delta-relaxation of DNA[2]. We also observe dielectric relaxations in a case of calculating time-correlation function with DNA and water molecules and ions,

which shows superposition of dielectric relaxations of DNA and bulk-like water around 50MHz and 10GHz, respectively.

These results are promising for further analysis on DNA electrical characteristics based on simulation, as well as theoretical calculations and measurements.



(a) Permittivity (b) Conductivity

Figure 1: Frequency-dependent permittivity and conductivity, which are the real part of the dielectric function and the imaginary part of the dielectric function, respectively.

Table 1: Simulation conditions

Force field	Lennard-Jones 12-6 potential (amber 94 parameter set)
System size	3.107 x 3.107 x 4.350[nm^3]
Molecules	8-mer random sequence DNA, 1239 water molecules, 16 Na^+, 2 Cl^-, Total 4244 atoms
Temperature	298[K] fixed
Time step	1[fs]
Cutoffs	Lennard-Jones: 0.9[nm], Ewald: 0.9[nm]
Simulation period	600[fs] for equilibrium, 7.3[ns] for correlation function

[1] S. Chowdhuri and A. Chandra, J. Chemical Physics, V. 115, No. 8, pp. 3732-3741, 2001.

[2] B.Saif, R.K.Mohr, C.J.Montrose, and T.A.Litovitz, Biopolymers, V.31, pp. 1171-1180, 1991