Thermal Conductivity of B-DNA

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ABSTRACT: The thermal conductivity of B-form double-stranded DNA (dsDNA) of the Drew–Dickerson sequence d(CGCGAATTCGCG) is computed using classical molecular dynamics (MD) simulations. In contrast to previous studies, which focus on a simplified 1D model or a coarse-grained model of DNA to reduce simulation times, full atomistic simulations are employed to understand the thermal conduction in B-DNA. Thermal conductivities at different temperatures from 100 to 400 K are investigated using the Einstein–Green–Kubo equilibrium and Müller–Plathe non-equilibrium formalisms. The thermal conductivity of B-DNA at room temperature is found to be 1.5 W/m·K in equilibrium and 1.225 W/m·K in the non-equilibrium approach. In addition, the denaturation regime of B-DNA is obtained from the variation of thermal conductivity with temperature. It is in agreement with previous studies using the Peyrard–Bishop–Dauxois model at a temperature of around 350 K. The quantum heat capacity (C_{vq}) has given additional clues regarding the Debye and denaturation temperature of 12-bp B-DNA.

INTRODUCTION

Probing thermal conduction in shorter length scales using computations gives us a fundamental understanding of the link between structure and phenomena with respect to heat transfer. DNA satisfies the low thermal conductivity requirements for building molecular thermoelectric devices.¹ This was a motivation for this study. In an experiment to find the thermal conduction of the DNA–gold composite where λ -DNA was coated with gold nanoparticles,² the thermal conductivity (κ) was found to be 150 W/m·K. Later studies have cited that gold primarily contributes to this high value of thermal conductivity, as the DNA contribution to the DNA–gold composite is less significant because of its ultra-low thermal conductivity.^{3–5} An experiment using a new transient electro-thermal technique with crystalline DNA composite fibers in NaCl solution has suggested that this might indeed be the case as the thermal conductivity found for the fibers is low at around 0.25–0.85 W/m·K.^{3,4}

Earlier computational studies use the Peyrard–Bishop–Dauxois (PBD) model, which is a simplified 1-D non-linear bead spring model.⁶ This model has been used to understand DNA dynamics and to find the denaturation point of DNA.⁷ The denaturation regime of DNA was found to be around 350 K and the thermal conductivity of the DNA at 300 K is 1.8 mW/m·K.⁸ This value is much lower than that of poly(G) DNA (≈ 0.3 W/m·K) obtained using a 12-coarse-grained model.⁵ The disagreement raises the question of the validity of thermal conductivity computed using the PBD model. A few infinite chains formed by permuting adenine (A) and guanine (G) sequences—poly(A), poly(G), poly(AG), poly(A₂G₂), and poly(A₂₀₀G₂₀₀)—are investigated using the PBD model and it was found that the denaturation point can be shifted

depending on the sequence.⁹ Additionally, the thermal conductance ratio $R = \kappa_H/\kappa_L$, which is defined as a high thermal conductivity to a low thermal conductivity of various sequences, is quantified to analyze thermal switching in DNA. The sequence poly(A₂G₂) seemed to have a higher thermal conductance ratio than poly(A) and poly(G) sequences. Again, the thermal conductance values were extremely lower, probably owing to the PBD model.⁹ The PBD model has also been used to understand the improving of heat conduction through external force.¹⁰ As an extension of this, DNA switching was studied by considering one end of the DNA helical turn as a drain, another end as a source, and the central region as a gate.¹¹ An all-atom picture resolves the discrepancies in understanding the fundamental nature of thermal conduction in a DNA. Hence, the water and Na⁺ ions are considered as the stabilizing media and only the thermal conductivity of B-DNA is calculated.

COMPUTATIONAL DETAILS

All the calculations are performed on the 12-base-pair (bp) B-DNA of Drew–Dickerson sequence d(CGCGAATTCGCG).¹² A nucleic acid builder module of AMBERTOOLS18¹³ is used to build the initial structures of the double-stranded (ds) DNA. The dsDNA is then placed in a bath of TIP3P water box¹⁴ using an xleap module of the

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AMBERTOOLS18 software package. A water box with dimensions of $65 \text{ \AA} \times 65 \text{ \AA} \times 90 \text{ \AA}$ ($x \times y \times z$) is chosen to ensure a $15 \text{ \AA}$ solvation shell around the B-DNA. Twenty-two Na^+ ions are added at the lowest electrostatic potential locations to the solvated dsDNA system. A DNA OL15 force-field¹⁵ is used. This has parmbsc0¹⁶ and OL15¹⁵ corrections to the ff99 force-field¹⁷ to consider the bonded and non-bonded interactions of the dsDNA. The Joung–Cheatham parameter¹⁸ set is used to consider the interaction of monovalent Na^+ ions with TIP3P water and dsDNA (Figure 1).

Figure 1. The simulated B-DNA structure is in a water box with Na^+ ions. The B-DNA has a total length of $40.8 \text{ \AA}$, a radius of $10 \text{ \AA}$, and is colored according to different atom types. Also shown is the non-equilibrium Müller–Plathe scheme where the red region with the higher temperature swaps kinetic energies with the blue regions with lower temperatures.

After preparing the initial system using AMBERTOOLS18, a LAMMPS¹⁹ software module is used for all further simulations. The whole solvated dsDNA system is energy-minimized using first 5000 steps of steepest descent and 5000 steps of conjugate gradient, keeping the B-DNA restrained with a force of $500 \text{ kcal/mol \AA}$. The DNA is then slowly released into water by reducing the restraint from $20 \text{ kcal/mol \AA}$ to $0 \text{ kcal/mol \AA}$ in five cycles of the steepest descent and conjugate gradient minimization steps. All the atoms are then assigned velocities according to a Maxwell–Boltzmann distribution. Throughout the MD simulation, the DNA has a small restraint of $1 \text{ kcal/mol \AA}$ to prevent the same from changing its orientation while measuring the thermal conductivity. SHAKE constraints²⁰ are applied to the hydrogen atoms, bond, and angles of DNA and water with a tolerance of 10^{-4} . The system is equilibrated for 10 ns with a Nosé–Hoover thermostat and barostats with coupling constants for 0.1 and 1.0 ps , respectively.^{21–24} Finally, a production run of 20 ns for the calculation of thermal conductivity ensures that the thermal conductivity values converge. The thermal conductivity is computed using the equilibrium Green–Kubo (GK) method, where the heat–heat auto-correlation function is used to compute the thermal conductivity as^{25–27}

$$\kappa_{x,y,z} = \frac{V}{k_B T^2} \int_0^\infty \langle J_{x,y,z}(0) \cdot J_{x,y,z}(t) \rangle dt \quad (1)$$

where thermal conductivity $\kappa_{x,y,z}$ at a temperature T in a direction x , y , or z is obtained from heat current $J_{x,y,z}$ in that direction. k_B is the Boltzmann constant. The heat current is obtained as

$$J = \frac{1}{V} \left[\sum_i e_i v_i - \sum_i \sigma_i v_i \right] \quad (2)$$

where e_i is the total energy of an atom, v_i is the velocity of an atom, σ_i is the virial stress per atom, and V is the volume of the total group of atoms. The exact volume (V) of B-DNA is

computed from the atomic volumes of adenine ($136.1 \text{ \AA}^3$), guanine ($143.8 \text{ \AA}^3$), cytosine ($113.2 \text{ \AA}^3$), and thymine ($132.6 \text{ \AA}^3$) base-pair groups and sugar-phosphate ($174.8 \text{ \AA}^3$) groups. These atomic volumes are computed by the radical planes method on experimental DNA datasets.^{28,29} Each strand (left or right of B-DNA symmetrical axis) contains four cytosine, four guanine, two adenine, two thymine, and 12 sugar-phosphate groups, giving us the total volume (V) of the 12-bp B-DNA to be $7326 \text{ \AA}^3$. The power spectrum density or density of states (DoS) of the 12-bp B-DNA is obtained from a fast Fourier transform of velocity–velocity auto-correlation, $C(t)$, as

$$\text{DoS}(\nu) = \lim_{t \rightarrow \infty} \frac{1}{2k_B T} \int_{-\tau}^{\tau} C(t) e^{-2\pi\nu t} dt \quad (3)$$

where t is the correlation time window of 200 ps and ν is the frequency. Only the solid component of DoS is considered as liquid and gaseous states are not relevant for B-DNA. The canonical partition function (Q) can be constructed from DoS, with a harmonic oscillator assumption^{30–32}

$$\ln Q = \int_0^\infty \text{DoS}(\nu) q_{\text{HO}}(\nu) d\nu \quad (4)$$

where $q_{\text{HO}} = \frac{e^{-\beta h \nu}}{1 - e^{-\beta h \nu}}$ is the harmonic oscillator partition function, $\beta = \frac{1}{k_B T}$, and h is Planck's constant. The entropy S^0 and the heat capacity C_{vq} are then found using the partition function and DoS as

$$\begin{aligned} S^0 &= k \ln Q + \beta^{-1} \left(\frac{\partial \ln Q}{\partial T} \right)_{N,V} \\ &= k \int_0^\infty \text{DoS}(\nu) W^s(\nu) d\nu \end{aligned} \quad (5)$$

$$\begin{aligned} C_{vq} &= \left(\frac{\partial S^0}{\partial T} \right) \\ &= k \left(\frac{\partial \ln Q}{\partial T} \right)_{N,V} + \beta^{-1} \left(\frac{\partial^2 \ln Q}{\partial T^2} \right)_{N,V} \\ &= k^2 \beta^{-2} \int_0^\infty \text{DoS}(\nu) W^c(\nu) d\nu \end{aligned} \quad (6)$$

with weighting functions

$$W^s(\nu) = \frac{\beta h \nu}{e^{\beta h \nu} - 1} \ln[1 - (e^{-\beta h \nu})] \quad (7)$$

$$W^c(\nu) = \frac{e^{-\beta h \nu}}{[1 - (e^{-\beta h \nu})]^2} \quad (8)$$

RESULTS AND DISCUSSION

Thermal Conductivity Using the GK Equilibrium Method. The thermal conductivity of B-DNA is calculated using the equilibrium GK method as in 1. This requires the calculation of the heat–heat auto-correlation function from heat current using eq 2, and this settles to an equilibrium value. The thermal conductivity value was obtained at 300 K along the length of the DNA after it had settled to an equilibrium value for 10 ns (Figure 2). All equilibrium GK thermal conductivity values at different temperatures are obtained

Figure 2. Convergence of thermal conductivity of B-DNA at 300 K along the length of the DNA in GK.

similarly. The thermal conductivity of the dsDNA sequence along its length as a function of temperature is shown in Figure 3. The thermal conductivity increases as a function of temperature and eventually saturates at around 350 K.

Figure 3. Equilibrium GK thermal conductivities of B-DNA along the length of the DNA as a function of temperature.⁴

The equilibrium method also allows us to calculate the heat flux along the other directions such as those between the strands, as shown in Figure 4. These thermal conductivities are

Figure 4. Equilibrium GK thermal conductivities of B-DNA along base pairs κ_y as a function of temperature.

inaccessible to experiments at such shorter strand lengths. Interestingly, the heat transfer along base pairs between the backbone is higher than that along the strand. No parallels exist in reported literature about the heat conduction between strands, although it has been mentioned that the heat conduction along the length is primarily due to sugar-phosphate backbone.⁵ The classical treatment here has not accounted for the transfer of heat between base pairs by tunneling. Nevertheless, it is evident from Figure 4 that more heat can be transferred along base pairs than along the length of the phosphate backbone.

Thermal Conductivity Using the Reverse Non-equilibrium MD Method. A non-equilibrium MP approach³³ is also used to understand the low thermal conductivity obtained earlier using equilibrium formulation. Here, a temperature gradient was set along the length of B-DNA and the surrounding water box by swapping kinetic energies every step with the box being divided into 100 chunks in the z -direction. The temperature profile across the surrounding water clearly has a gradient between the center hot region and cold regions on either side. Figures 5 and 6 show the water and DNA temperature profiles, respectively.

Figure 5. Temperature profile across the water box, which has B-DNA along the z -direction.

Figure 6. Temperature profile across the 12-bp B-DNA in the RNEMD simulation along the z -direction.

The thermal conductivity κ due to a linear temperature gradient between the DNA ends (between 22.5 and 67.5 Å) is given as

$$\kappa_z = \frac{\left(\frac{Q}{At}\right)}{(\partial T/\partial z)} \quad (9)$$

where Q is the heat exchange between hot and cold regions, A is the cross-sectional area of the water box, and t is the time for heat exchange. Also, note that the Q value above is already divided by 2 as heat flows from the center hot chunk to two cold chunks in two directions. The temperature gradient in eq 9 is computed only across B-DNA from a smoothened temperature profile in Figure 6 in the convergent regime (Figure 7). Caution was exercised in calculating the temper-

Figure 7. Convergence of thermal conductivity of B-DNA at 300 K along the length of the DNA in RNEMD simulation.

ature profile as constrained SHAKE atoms were excluded and a mild Berendsen thermostat with damping constant of 10,000 timesteps was used.³⁴ Figure 8 shows the temperature dependence of the thermal conductivity using this method and the profile similar to GK thermal conductivity (Figure 3).

Power Density Spectrum. To understand the molecular origin of the temperature dependence of the thermal conductivity of the DNA, the DoS of the 12-bp B-DNA have been calculated using a 2-point (2pt) code^{30–32} and have been plotted in Figure 9. Only continuous low-frequency modes can

Figure 8. Thermal conductivities versus temperature for 12-bp B-DNA in RNEMD simulation.

Figure 9. Power spectrum density of B-DNA at 300, 100, and 400 K.

be seen till 800 cm^{-1} (Debye frequency, ω_D). In an earlier study on poly-G DNA,⁵ the DoS spectrum had a gap with no modes between 200 and 300 cm^{-1} . Moreover, few modes existed beyond this gap till 400 cm^{-1} . No such gap is seen in the spectrum between optical and acoustic modes. No high-frequency modes have been observed in both this study and in an earlier study,⁵ meaning that the phonon modes have large wavelengths and hence are scattered at the dsDNA boundaries. Around the denaturation temperature, the DNA strands separate, and the thermal conductivity saturates. It is possible to compute the Debye temperature, T_D , from this spectrum by using $T_D = \hbar\omega_D/k_B$, where $\hbar$ and k_B are reduced Planck's constant and Boltzmann constant, respectively. Substituting ω_D to be 723 cm^{-1} as it is the last available frequency mode, $T_D \approx 165$ K.

Using the DoS shown in Figure 9, also computed is the quantum molar specific heat capacity (C_{vq}) of the dsDNA (Figure 10a). The resulting heat capacity is plotted as a function of temperature. The peaks in heat capacity at 200 and 273 K in Figure 10a are probably due to water as similar features can be seen in water heat capacity at the same temperatures in Figure 11. The peak at 150 K is close to the calculated Debye temperature (165 K) of DNA. The peak around 350 K (Figure 10b) ought to correspond with the denaturation regime, where the transition from a double strand to two single strands happens.³⁵ It is till this point that the thermal conductivity increases and beyond which thermal conductivity saturates. A similar study⁸ has described the same phenomenon and it is mentioned that the increase in thermal conductivity is strongly correlated with the anharmonicity in the bond between the complementary base pairs till there is effectively no contact between the complementary base pairs.

Till denaturation, there is an increase in thermal conductivity κ and quantum heat capacity (C_{vq}) of B-DNA with respect to temperature. This is attributed to increase of phonon density with respect to temperature⁴ as $\kappa = \frac{C_v^2 \tau_r}{3}$ in the single time relaxation approximation. Moreover, it can be seen from Figure 9 that only low-frequency (long wavelength) soft modes are available in DNA, allowing this classical approximation to be valid. The heat capacity (C) of B-DNA also increases initially with temperature as the Debye law states: $C_{vq} \propto T^3$ (refer Figure 10a). It is being assumed that the phonon velocity (v) remains almost constant with temperature and the relaxation time $\tau_r \propto T^{-1}$.⁴ Hence, the thermal conductivity initially increases almost quadratically with

Figure 10. (a) Quantum heat capacity (C_{vq}) of B-DNA as a function of temperature and (b) inset of data around the mentioned denaturation temperature (T_m) for clarity.

Figure 11. Quantum heat capacity (C_{vq}) of TIP3P water as a function of temperature.

respect to temperature till the DNA strands separate. The thermal conductivity of the DNA–gold composite is found to be $150 \text{ W/m}\cdot\text{K}$,² whereas recent estimates of the thermal conductivity of the DNA–water composite mixture via equilibrium and non-equilibrium MD were 0.381 and $0.373 \text{ W/m}\cdot\text{K}$, respectively.³⁶ Our results suggest that there is a definite contribution of gold and water to the thermal conductivity of the composite mixture in these studies and

the thermal conductivity of DNA is somewhere close to the reported values in this study.

CONCLUSIONS

The thermal conductivity of 12-bp B-DNA, the most common form of DNA, was examined from GK and reverse non-equilibrium molecular dynamics (RNEMD) calculations. Both calculations have shown an increase in thermal conductivity till denaturation temperature. The full atom description, as opposed to coarse-grained or 1D non-linear chain models, indicates the regions where the models succeed and fail. The thermal conductivity obtained using PBD models needs to be refined as they seem to be very low. Nevertheless, all models predict the denaturation regime close to 350 K , where the thermal conductivity saturates with increase in temperature. One should also note that the full-atom thermal conductivities are also dependent on force-field used. The 2pt calculations show that the Debye temperature is consistent with earlier studies.^{5,8,9} The thermal conductivity of one sequence has been studied. The engineering of thermal conductivity, based on the various base-pair sequences along the long lengths, might play a role in its usage as a molecular thermoelectric device operating at room temperature. This study lays the foundation for an all-atom study of DNA thermal conductivity. Building further using the methods here would give us insights into the dependence of thermal conductivity on base-pair sequences from an all-atom perspective. The thermal conductivity computed here might be a necessary validity check for coarse-grained DNA models.

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Notes

The authors declare no competing financial interest.

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