

Effect of Water Molecules at Different Temperatures on Properties of Cellulose Based on Molecular Dynamics Simulation

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Six hybrid models of cellulose amorphous region and water molecules were established by using a molecular dynamics software to simulate changes of cellulose and water molecules during bamboo hydrothermal treatment. The results indicated that in the range of hydrothermal treatment temperature of bamboo from 150 to 240 °C, the diffusion coefficient of water molecules increased with the increase of temperature, conducive to the processing efficiency of hydrothermal treatment. The mean square displacement (MSD) of the bamboo cellulose chain increased with the increase of temperature, not conducive to the thermal stability of cellulose. The energy change of the system predicts that a higher hydrothermal treatment temperature will result in faster material aging degradation. The comprehensive analysis of mechanical parameters showed that when the hydrothermal treatment temperature did not exceed 180 °C, bamboo cellulose had better plasticity and toughness.

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Keywords: Bamboo heat treatment; Molecular dynamics; Diffusion coefficient; Energy change; Mechanical properties

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INTRODUCTION

Bamboo is a natural material with a short production cycle and high mechanical strength, which has great development potential (Sharma *et al.* 2015). Bamboo is widely used in decoration, architecture, furniture, and many other fields (Asif 2009; Febrianto *et al.* 2012; Qi *et al.* 2014; Sun *et al.* 2020). However, bamboo also has many disadvantages, including its low natural durability and the fact that its size tends to change if the environment changes (Colla *et al.* 2011). Because bamboo is made up of cellulose, hemicellulose, sugars, proteins, and starch, it is prone to mildew, cracking, and moth-eating problems (Liese 1980; Liese 2003). Therefore, the modification of bamboo has a strong practical significance.

Heat treatment can be used to improve the performance of bamboo products (Tao *et al.* 2015). Bamboo heat treatment is similar to wood heat treatment. It uses air, inert gas, or steam as a heat transfer agent for physical modification treatment at high temperatures between 150 to 240 °C. Heat treatment improves the physical properties, dimensional stability, and hygroscopicity of bamboo because of the change of surface and internal structure and composition of bamboo (Cao *et al.* 2012; Wang *et al.* 2018). Appropriate treatment temperature reduces the hygroscopicity and water absorption of bamboo and

improves the dimensional stability and durability of bamboo. The high temperature leads to surface hardening and reduces its mechanical strength, which reduces the comprehensive strength of bamboo and affects its application in bamboo products and the bamboo industry (Yang *et al.* 2016; Azadeh and Ghavami 2018). Different treatment temperatures have a significant effect on the properties of bamboo after hydrothermal treatment.

Many studies have revealed the effect of temperature on the properties of bamboo. Bui *et al.* (2017) found that bamboo has the best durability and mechanical properties when the temperature is 180 °C and the treatment time is 1 to 2 h. Wang *et al.* (2020c) reported that high temperature saturated steam treatment reduces the equilibrium moisture content of bamboo and improves the dimensional stability and durability of bamboo stalks; the 180 °C treatment for 10 min is a favorable treatment condition. Wang *et al.* (2020a) found that the compressive strength, bending strength, and bending elastic modulus of bamboo are increased, while the shear strength is decreased when the temperature is 180 °C.

Hydrothermal treatment can improve the properties of bamboo. Studies have shown that the heat treatment of bamboo in water vapor at suitable temperature can improve the dimensional stability and durability of bamboo. But temperature that is too high will reduce its mechanical strength. Therefore, it is important to find the right hydrothermal treatment temperature.

With the development of heat treatment and molecular dynamics technology, the research on cellulose from the microscopic level of bamboo has gradually become a hotspot of research. Khazraji and Robert (2013) found that the cellulose polymer has strong reactivity with water molecules, and water molecules easily form a hydrogen bonds with the cellulose chain. Huang *et al.* (2019) revealed that ammonia molecules increase the end distance of cellulose I β and thus enhance its compliance. Wang *et al.* (2020b) found that the mass fraction of water molecules has a greater impact on bamboo heat treatment through molecular dynamics simulation, and cellulose has the best mechanical properties when the mass fraction of water was 3% for heat treatment simulation.

While it is common to study the interaction between cellulose and small molecules from the microscopic point of view, there have been few reports on the effect of temperature on the related properties of bamboo hydrothermal treatment. The goal of this work was to study the effect of water molecules on the mechanical properties of cellulose in the process of bamboo hydrothermal treatment at different temperatures from a microscopic perspective. An attempt is made in this work to find a suitable range of temperature during hydrothermal treatment of bamboo, to provide relevant theoretical support for bamboo hydrothermal treatment.

EXPERIMENTAL

Method

Modeling

Cellulose, the main component of bamboo, is a polymeric compound formed by the polymerization of D-glucopyranose. It consists of crystalline and amorphous regions. The cellulose molecules in the crystalline zones are arranged in a compact and orderly manner, and their mechanical properties are difficult to be broken at high temperatures. However, the amorphous region of cellulose has an irregular structure and good flexibility, which can make the cellulose material show a soft side, and its mechanical properties are easily affected by temperature (Khazraji and Robert 2013). Therefore, the amorphous region was

selected to study the effect of temperature on bamboo hydrothermal treatment.

The amorphous region of the bamboo cellulose molecular chain was modeled using Materials Studio 8.0 software (BIOVIA, v.8.0, San Diego, CA, USA). The degree of polymerization (DP) has no remarkable effect on the simulation results of the physical properties of the material (Mazeau and Heux 2008). In this paper, a cellulose chain was created with a DP of 20 (Wang *et al.* 2018). The construction of the amorphous region polymer adopts the method proposed by Theodorou and Suter (1985) and uses the Amorphous Cell Tools (AC) module for modeling. The model target density was set to 1.5 g/cm³ (Onyon 1972). In the model, 30 water molecules and a cellulose chain with a DP of 20 were added. The size of the simulated unit cell was 20.2 × 20.2 × 20.2 (Å³). The established model is shown in Fig. 1.

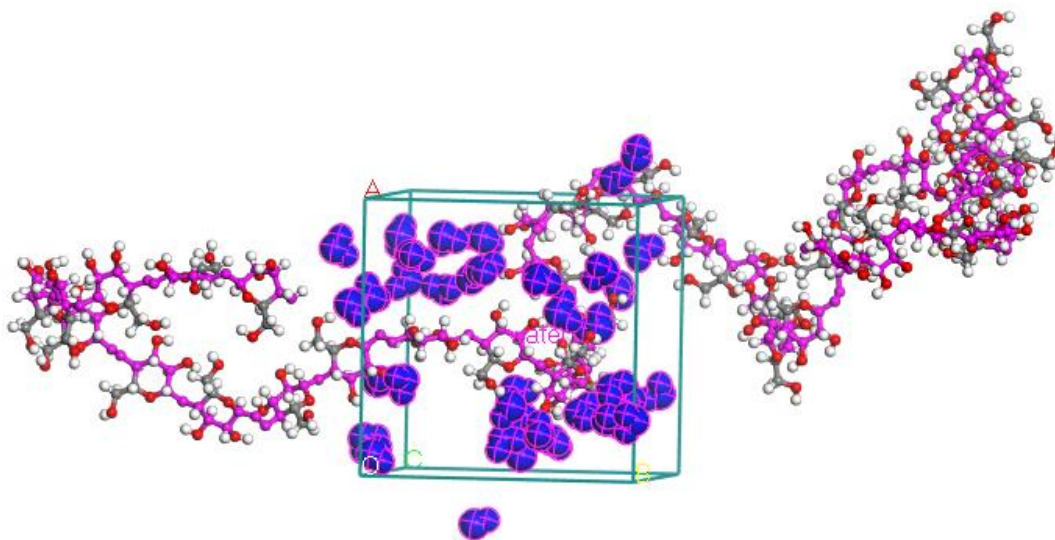


Fig. 1. Cellulose amorphous region-water model. The red chain is a bamboo cellulose molecular chain, and the blue spheres are water molecules.

Dynamic simulation

The model shown in Fig. 1 was optimized for structure and energy minimization. The Forcite Calculation module was used for structural optimization, and the smart algorithm was chosen to run 5000 steps. The dynamic relaxation of the model was carried out at 25 °C in the canonical ensemble (NVT) for 1000 ps to minimize the energy of the system. The time step was 1 ps. One frame was output every 5000 steps, and the Nose method was selected as the temperature control method. The temperature of bamboo hydrothermal treatment starts from 90 °C and increases by 30 °C each time to 240 °C. This temperature range includes the set temperature required for the bamboo hydrothermal treatment process.

The dynamic simulation was of the model carried out in the isothermal isobaric ensemble (NPT) with a time of 1000 ps. The Andersen method was selected as the temperature control method (Andrea *et al.* 1983); the Berendsen method was selected as the pressure control method (Berendsen *et al.* 1984). The Van der Waals force was computed by atom-based calculations (Andersen 1980); the electronic effect was computed by the Ewald method (Ewald 1921). All simulations were performed under the PCFF force field, which originated from the CFF91 force field. It is suitable for calculating organic compounds, especially natural polymer materials.

RESULTS AND DISCUSSION

The Energy

In molecular dynamics simulation, energy was used as the basis for system equilibrium. Figure 2 shows the dynamic energy diagram of the bamboo cellulose-water molecule model. The total energy values of the last 200 ps fluctuated slightly above and below its average value, which showed that the system tends to equilibrium.

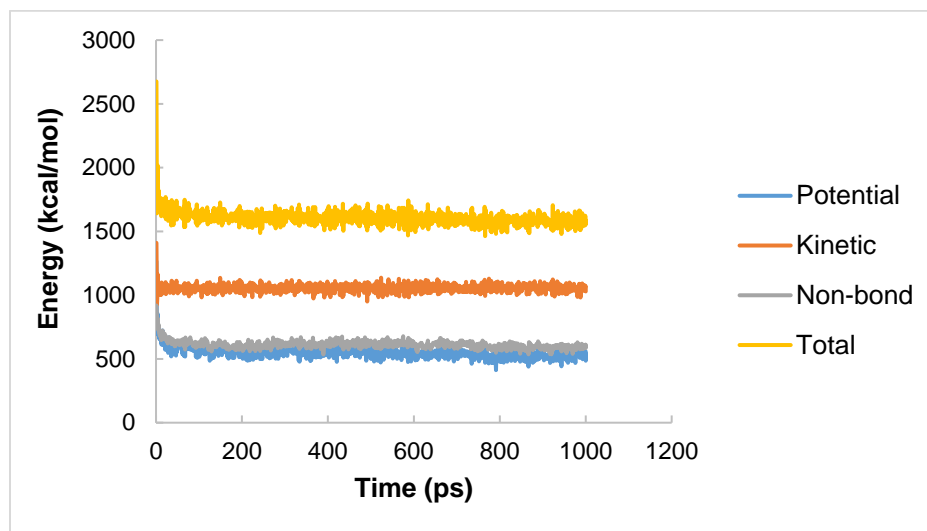


Fig. 2. The dynamics energies of model

In Fig. 2, Potential represents total potential energy, Kinetic represents kinetic energy, Non-bond represents non-bond energy term, and Total represents total energy. The non-bond energy term includes electrostatic interaction and van der Waals interaction. In this paper, the PCFF force field is selected, and its total potential energy expression is more complicated (Sun 1995; Maple *et al.* 2013). It can be simply expressed as Eq. 1,

$$E_{total} = E_{cross} + E_{internal} + E_{nonbond} \quad (1)$$

where $E_{nonbond}$ is the non-bond energy term, and $(E_{cross} + E_{internal})$ is the sum of the potential energy of the water molecule and the cellulose molecule, called the bond energy term. The total potential energy of the system is equal to the sum of non-bond energy term and bond energy term. In the simulation process, as the temperature increases, when the total potential energy exceeds the non-bonded energy term, the bond energy term changes from a negative value to a positive value. That means covalent bonds are becoming more unstable. As the heat energy increases, the bond energy term increases and the covalent bond becomes unstable. Some active bonds in the bamboo material are unstable or even broken, which leads to bamboo cellulose aging and degradation.

As shown in Fig. 3, the mean value of the non-bond energy term and the mean value of the total potential energy showed a linear increasing trend with increased temperature; when the temperature was greater than 120 °C, the mean value of the total potential energy gradually became larger than the mean value of the non-bond energy term. The mean value of the bond energy term changes from negative to positive. The bond energy is the difference between the total potential energy and the non-bond energy, as shown in Table 1.

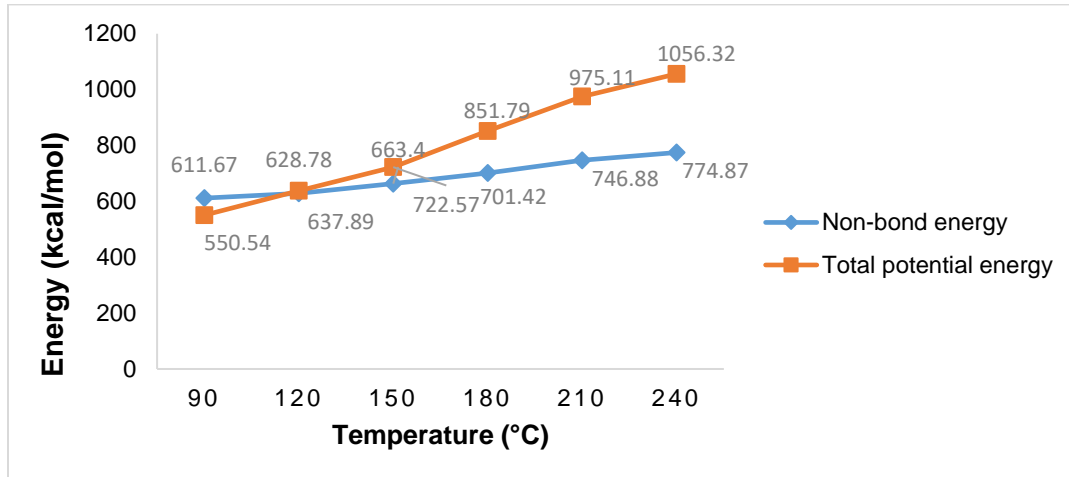


Fig. 3. The average energies of the model at different temperatures

Table 1. The Average Bond Energy of the Model at Different Temperature

Temperature (°C)	150	180	210	240
Bond-energy (kcal/mol)	59.17	150.37	228.23	281.45

The bond energy term increased continuously with the increasing temperature. According to these data, temperature damages bamboo fiber. Therefore, to meet the basic temperature requirements of hydrothermal treatment, the temperature should be lowered as much as possible to reduce the influence of temperature on bamboo.

Diffusion Coefficient of Water Molecules

The diffusion coefficient is an important parameter that reflects the ability of small molecules to diffuse in a substance. The size of the diffusion coefficient can be calculated by the mean square displacement (MSD). The MSD refers to the mean square sum of the vector increment of the water molecule position after the dynamic simulation, as represented by Eq. 2,

$$\text{MSD} = \sum_{i=1}^n \left\langle \left| \vec{r}_i(t) - \vec{r}_i(0) \right|^2 \right\rangle \quad (2)$$

where $\vec{r}_i(t)$ and $\vec{r}_i(0)$ represent the displacement of the atom i at time t and time 0. The diffusion coefficient (D) is usually expressed by Eq. 3 (Einstein 1905; Brown *et al.* 2010),

$$D = \frac{1}{6N_w} \lim_{t \rightarrow \infty} \frac{d}{dt} \sum_{i=1}^n \left\langle \left| \vec{r}_i(t) - \vec{r}_i(0) \right|^2 \right\rangle \quad (3)$$

where N_w is the number of water molecules in the system. The Einstein relationship can be used to solve the diffusion coefficient by the slope of the mean square displacement when t is large enough (Yang *et al.* 2013), as shown in Eq. 4,

$$D = K / 6 \quad (4)$$

where K represents the slope of the mean square displacement (MSD) curve. Based on the analysis of the model, the MSD at different temperatures was obtained (Fig. 4).

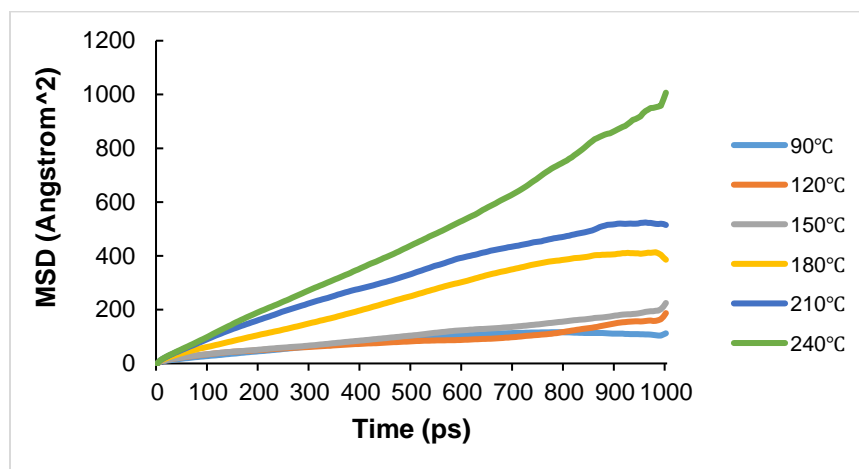


Fig. 4. Mean squared displacement curves of water at different temperatures

As shown in Fig. 4, the MSD of water molecules increased linearly with time in the simulation time of 0 to 900 ps, and there was a large deviation from 900 to 1000 ps. This deviation can be regarded as a statistical error calculation. The first 900 ps was fit according to the principle of the least square method to find the size of the diffusion coefficient, as shown in Table 2. The diffusion coefficient of the water molecule in the cellulose model increased with rising temperature; at higher temperatures, more energy is absorbed by water molecules. With the increase of its energy, the thermal motion of water molecules becomes more violent, which makes it easier to penetrate the bamboo cellulose chain, thereby improving the processing efficiency of bamboo hydrothermal treatment.

Table 2. Diffusion Coefficient D of Water at Different Temperatures

Temperature (°C)	90	120	150	180	210	240
The slope	0.1262	0.1219	0.1780	0.4678	0.5518	0.9239
Diffusion coefficient (A ² /ps)	0.0210	0.0203	0.0297	0.0780	0.0920	0.1540

The MSD of the Bamboo Cellulose Chain

There are five crystalline variants of cellulose in the solid-state, namely cellulose I, II, III, IV, and X. Cellulose I belongs to natural cellulose. It has two different crystalline phases, I α and I β . The former mainly exists in bacterial fibers and belongs to the triclinic unit cell model, while the latter mainly exists in animal fibers and higher angiosperms. It belongs to the monoclinic unit cell model (O'Sullivan 1997). Bamboo cellulose, wood cellulose, and cotton and linen fibers are all-natural cellulose and are derived from higher angiosperms, so their main component cellulose has similar structure and properties. The MSD of the bamboo cellulose chain can indicate the movement of the cellulose molecular chain. The violent movement of the bamboo cellulose chain determines its stability. More movement indicates decreased stability. Therefore, the stability of the overall bamboo structure is reduced. As shown in Fig. 5, the MSD of cellulose molecules increased linearly with time in the simulation time of 0 to 900 ps. Within the scope of 900-1000 ps curve appeared different degree of deviation, because the calculation includes the statistical error. In the temperature range of 90 to 150 °C, the MSD of the bamboo cellulose molecular

chain did not change significantly. In the temperature range of 180 to 240 °C, the MSD of the bamboo cellulose molecular chain increased with increasing temperature. Further analysis showed that when the hydrothermal treatment temperature was within the range 160 to 240 °C, the stability of bamboo cellulose decreased with increasing temperature.

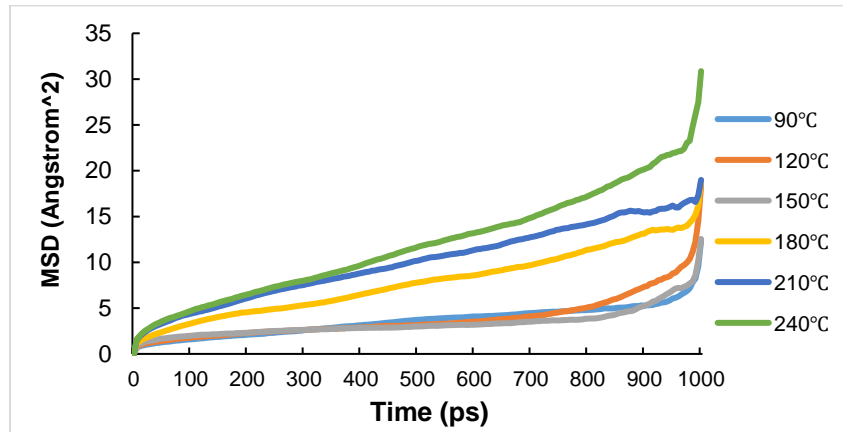


Fig. 5. Mean squared displacement curves of bamboo cellulose at different temperatures

Mechanical Properties

The dynamic mechanical parameters of the bamboo cellulose amorphous zone model at different temperatures characterize the effect of temperature on the changes in the mechanical properties of bamboo. Cauchy pressure (C12-C44) is usually used to measure the ductility of a system, which is the ability of a material to deform without cracking. The higher the value is, the better the ductility of the system is. In general, a material with good ductility will have a positive value (C12-C44); otherwise it will have a negative value. Young's modulus (E) is the longitudinal elastic modulus, which is used to characterize the ability of a material to resist deformation. A larger value indicates the ability of the material to resist deformation. Shear modulus (G) characterizes the ability of a material to resist shear strain, where a larger value represents stronger rigidity and less ductility. Poisson's ratio (γ) is the absolute value of the ratio of the material's transverse variable to the longitudinal variable when the material is subjected to external stress. A greater value results in stronger plasticity. The larger ratio of bulk modulus to shear modulus (K/G) indicates greater toughness in the material. The parameters of mechanical properties at different temperatures were obtained by the Forcite module in MS, and the results are shown in Table 3.

Table 3. Elastic Stiffness Constant of Cellulose Models at Different Temperature

Temperature (°C)	90	120	150	180	210	240
C12/(GPa)	5.7210	12.8800	11.4418	12.0747	11.2857	12.5306
C44/(GPa)	7.4514	5.4526	5.7420	5.1953	5.2535	5.2200
C12-C44/(GPa)	-1.7304	7.4274	5.6998	6.8794	6.0322	7.3106

When the treatment temperature is 90 °C, the Cauchy pressure is negative, indicating that the ductility of the system is poor. However, with the increase of temperature, the value of Cauchy pressure increased significantly and showed an increasing trend after 150 °C, indicating that the ductility of the system was good and had

a better and better trend. The authors believe that this is due to the low temperature at 90 °C and the weak interaction between water molecules and cellulose, which results in poor ductility. With the increase of temperature, the interaction between water molecules and cellulose becomes more intense, which increases its ductility. An extreme value appears at 120 °C, which may be because the non-bond energy is the closest to the total potential energy and the bond energy is the smallest, leading to the system in an equilibrium state.

The parameters λ and μ are called Lamé constants. They can be calculated by the Forcrite module. Lamé constants can be used to calculate Young's modulus (E), shear modulus (G), Poisson's ratio (γ), bulk modulus (K), as follows,

$$E = \frac{\mu(3\lambda + 2\mu)}{\mu + \lambda} \quad (5)$$

$$G = \mu \quad (6)$$

$$K = \lambda + \frac{2\mu}{3} \quad (7)$$

$$\gamma = \frac{\lambda}{2(\lambda + \mu)} \quad (8)$$

As shown in Table 4, with increasing temperature, the value of Young's variable with the boundary of 180 °C decreased first and then increased. Thus, the flexibility of bamboo material increased first and then decreased. Similarly, the value of shear modulus was smaller at 180 °C; with increasing temperature, the ductility at 180 °C decreased first and then increased. The values of Poisson's ratio and K/G were higher than other setting temperatures at 180 °C, but if the temperature continues to rise, the Poisson's ratio and K/G values gradually decreased. When the treatment temperature is below 180 °C, due to the increase of temperature, the interaction between water molecules and cellulose becomes more and more sufficient, leading to the mechanical properties of bamboo gradually becoming better. With the increase of temperature, the intermolecular bond energy gradually increases. When the temperature exceeds 180 °C, some active bonds in the bamboo material are unstable or even broken due to the large repulsive force between the atoms within the molecule, which leads to the deterioration of the mechanical properties of the bamboo cellulose. At 120 °C, the mechanical properties of cellulose are also better, which may be attributed to the lowest bond energy term in the system and the equilibrium state.

The simulation results are consistent with good plasticity when the heating temperature does not exceed 180 °C. Overall, these results indicate that if bamboo heat treatment is to pursue better plasticity, toughness, and ductility in the process of selecting water vapor as the heat transfer medium, the temperature setting of bamboo hydrothermal treatment should not exceed 180 °C. It is also consistent with the conclusion that hydrothermal treatment at appropriate temperature can improve the bending elastic modulus of bamboo, and too high temperature will degrade its properties, which Yun *et al.* (2016) studied.

Table 4. Mechanical Parameter of the Model at Different Temperatures

Temperature (°C)	λ	μ	Elastic Modulus (G/Pa)	Poisson's Ratio	K/G	Shear Modulus (GPa)
90	7.4761	6.8973	17.3821	0.2601	1.7506	6.8973
120	10.2052	5.6152	14.8526	0.3229	2.4841	5.6152
150	9.1430	6.1390	15.9509	0.2991	2.1560	6.1390
180	13.0238	4.6524	12.7327	0.3684	3.4660	4.6524
210	6.8907	6.3920	16.0910	0.2594	1.7447	6.3920
240	10.9757	5.9484	15.7545	0.3243	2.5118	5.9484

CONCLUSIONS

1. When the temperature of the simulated system is greater than 120 °C, the total potential energy of the system begins to exceed the non-bond energy term, and the bond energy term gradually increases. As a result, the covalent bonds become unstable and the bamboo fiber begins to age and degrade.
2. The diffusion coefficient of water molecules gradually increases with the increase of the hydrothermal treatment temperature. As the temperature rises, water molecules absorb energy to increase their energy, leading to accelerated thermal movement of water molecules, which is more conducive to improving the diffusion coefficient and water molecules entering the bamboo cellulose chain, thus improving the heat treatment processing efficiency of bamboo.
3. The mean square displacement (MSD) of the bamboo cellulose chain is easily affected when the temperature is greater than 150 °C. If the temperature is increased in the range of hydrothermal treatment temperature, then the thermal stability of the bamboo cellulose chain will decrease, which will affect the stability of bamboo cellulose.
4. The Cauchy pressure of bamboo cellulose changed from a negative value to a positive value with the increase of temperature, indicating that heat treatment was beneficial to the improvement of bamboo cellulose ductility. Simultaneously, the values of Young's variable and shear variable first decrease and then increase with the temperature increasing. Both have the minimum values at 180 °C and gradually increase when the temperature exceeds 180 °C. The values of Poisson's ratio and K/G first increase and then decrease, and have a maximum value at 180 °C, and gradually decrease when above 180 °C. These results suggest that if the goal for the heat-treated bamboo is to achieve better plasticity, toughness, and ductility, then the heat treatment temperature should not exceed 180 °C.

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