

Article

# MDPI

## Microcosmic Mechanism Investigation on Lightning Arc Damage of Wind Turbine Blades Based on Molecular Reaction Dynamics and Impact Current Experiment

## Li Zhang, Liyang Jiang \* 跑, Tong Zhao ២ and Liang Zou

School of electrical engineering, Shandong University, Jinan 250000, China; zhleee@sdu.edu.cn (L.Z.); zhaotong@sdu.edu.cn (T.Z.); zouliang@sdu.edu.cn (L.Z.)

\* Correspondence: jiangliyang85@gmail.com; Tel.: +86-182-5316-3345

Received: 10 October 2017; Accepted: 20 November 2017; Published: 1 December 2017

**Abstract:** PVC and balsa wood are usually used in the interlayer structures of wind turbine blades. In this paper, a comparative study on the lightning damage characteristics of the two materials was carried out by molecular dynamic simulations and impact current experiments. The simulations show that the glycosidic bonds in cellulose break first, which leads to a strong decrease in the degree of polymerization (DP) of cellulose (while the DP of PVC changes irregularly), then C–O bonds in the pyranoid ring break and the main chain of cellulose is destroyed, producing small molecule fractions and a lot of gas molecules. There are two steps in the pyrolysis of PVC. H and Cl atoms fall off the main chain and combined for form HCl, which needs less energy and occurs earlier than cellulose pyrolysis at 2000 K, but cellulose generates more gas products than PVC at the same temperature. Thus the damages to balsa wood and PVC mainly appear as fiber fractures and pore extension, respectively, which are consistent with the morphological features of the damage to the two materials in the impact current experiments. The experimental results also show that the pyrolysis temperature of PVC was lower than that of balsa wood, and the residual strength decreases faster in PVC than in balsa wood with the increase of peak current. This study should play an important guiding role for lightning protection and material selection of wind turbine blades.

**Keywords:** lightning protection; wind turbine blades; molecular dynamics; damage caused by lightning; balsa wood; PVC; pyrolysis

## 1. Introduction

Wind energy is one of the most promising renewable energies, and wind power generation has developed rapidly in recent years. The global installed wind power capacity in 2016 was 20 times that of 2001. With the increase of the wind turbine unit capacity and the wind farm scale, the hub height and blade length of wind turbines has increased, and most wind farms are located on open ground and mountains, so they are easily struck by lightning [1–3]. According to the US wind energy insurance claims report in 2012, the proportion of the damage caused by lightning was 23.4% of the turbine failures. Damage caused by lightning can occur in the blades, generators, controllers, control cables and other parts. Blades are the most vulnerable parts of the turbines, with the highest maintenance costs and the longest downtime (about 10 days after each accident). Although there are some flow control devices such as improved microtab system [4,5] to decrease damage and loads on wind turbine blades, these methods cannot protect the blades against lightning. At present, epoxy resin reinforced by glass fiber is mainly used in the spar cap of wind turbine blades, and the interlayer structure is usually made by PVC and balsa wood in order to reduce weight. However, these two materials are seldom compared in terms of their lightning damage characteristics.

When lightning strikes the blades, the instantaneous large current increases the electric field intensity in the internal pores of the material, triggering an avalanche of ionization of the dielectric, which forms a plasma discharge channel where the temperature rises rapidly to several thousand degrees Celsius in a brief time (1–5 µs). The blade materials decompose rapidly at high temperature, and the wind turbine failure will occur. It is pointed out in [6,7] that the lightning strike can produce a surface arc, which will go into the pores and the Joule heat will lead to a rapid temperature rise, causing material surface damage along the arc path, while the Joule heat can also cause thermal pyrolysis of the epoxy resin and gasification of fiber materials, which will lead to the material delamination phenomenon [8]; Kithi et al. [9] studied the thermal expansion of water vapor in the blades and found that the different water vapor distribution in different parts and different materials of the blades caused imbalanced damage of the blades under the effect of lightning arcs and high temperature. It can be seen from the above study, lightning strikes will lead to a chemical degradation of PVC and balsa wood, and cause the mechanical strength of the two materials to decrease. In addition, gas products and water vapor expansion at high temperature will also lead to additional material damage. However these studies are all qualitative and quantitative studies and in-depth analysis of the chemical degradation processes of PVC and balsa wood are needed to study the mechanical damage characteristics of the two materials.

With the improvement of computer calculation, microcosmic simulation has gradually became an effective method to study physical and chemical properties of materials. The reactive force field (ReaxFF) was put forward by Adri et al. in 2001 [10]. Atomic bonds are judged by the relationship between bond length, bond order, and bond energy. The bond angle and torsional force are defined as a function of bond order [10], which can effectively simulate the molecular reaction process. At present, the force field has been applied to oxidization of hydrocarbon compounds [11], polymer system [12-14], high-energy materials system for the manufacture of explosives and fuel [15–17], metal oxide system and transition metal catalyst system [18,19]. For example, Zhong et al. [20] studied the reaction characteristics of phenolic hydroxyl groups at the initial stage of pyrolysis of phenolic resin. Zeng et al. [21] studied the erosion behavior of polyvinylidene fluoride (PVDF) under the attack of oxygen atom. Li et al. [22] studied the melting process of  $\beta$ -white quartz under external electric field. Diao et al. [23] studied the thermal degradation of epoxy resin. It was found that water was the main product and the water generation process was also studied. It can be seen that dynamics analysis of molecular reaction can be used to simulate the chemical degradation process of polymer materials, which can help to reveal the damage characteristics of blade materials caused by lightning.

The damage characteristics of PVC and balsa wood caused by lightning arc thermal effect were compared in this paper by molecular reaction dynamics and impact current experiments. The chemical reaction process, the main gas products and their generation mechanism as far as the two materials are concerned, were studied quantitatively. Then impact current experiments were carried out, and the morphological features of the damage to the two materials in the experiments were used to verify the simulation results. The simulation and experiment results showed the different pyrolysis microcosmic mechanism and damage characteristics of balsa wood and PVC. This paper can provide theoretical support for lightning protection of wind turbine blades.

## 2. Molecular Simulation of Material Arc Damage

The mechanical damage of the material under lightning arc exposure is mainly caused by material pyrolysis, gas product expansion, and the internal air expansion. The damage mechanism of balsa wood and PVC caused by arc heating effect was studied by means of a molecular reaction dynamics simulation at a molecular level.

## 2.1. Modeling and Simulation of Balsa Wood and PVC

### 2.1.1. Molecular Model of PVC and Balsa Wood

The main components of PVC and balsa wood are polyvinyl chloride (PVC) and cellulose, respectively. In this paper, the two polymer molecules of different degree of polymerization (DP) were simulated. It was found that the DP has little effect on the pyrolysis process of the two macromolecules. Taking into account the convenience of observation and the calculation speed, the cellulose molecule with 2 DP and the PVC molecule with 4 DP were modeled and simulated to study the microscopic mechanism of pyrolysis. The periodic cells of the two molecules were built by Material Studio software. The periodic boundary condition was used to eliminate boundary effect. The target densities of the two models were 1.59 g/cm<sup>3</sup> (cellulose) and 1.35 g/cm<sup>3</sup> (PVC) respectively. The models of cellulose and PVC were shown in Figures 1 and 2. The carbon atoms are gray, oxygen atoms are red, hydrogen atoms are white, and chlorine atoms are green.



Figure 1. The model of cellulose with 2 DP.



Figure 2. The model of PVC with 4 DP.

## 2.1.2. Simulation Process

Because the lightning strike can lead to a temperature increase of thousand degrees Celsius in blades, material pyrolysis tests were carried out over a temperature range from 1000 K to 5000 K and it was found that the reactions under 4000 K were slow and incomplete, and when the temperature was 4000 K, the reaction was basically completed in 200 ps. Thus the simulation temperature was set to 4000 K and the reaction time was set to 200 ps.

## a. Model optimization

Firstly, energy minimization of the established model was performed; then the minimized cells were optimized according to their dynamic equilibrium at 298 K for 20 ps based on NVE, NPT, and NVT ensembles, respectively (N was the number of atoms V was the volume of the cell, T was the temperature of the cell, E was the energy of the cell and P was the pressure of the cell, for example, NVT ensemble was a system with constant atom number, volume and temperature). Each time the dynamic equilibrium optimization was completed, the energy of the system was minimized again.

## b. Pyrolysis reaction

The molecular dynamic reaction of the optimized model at 4000 K was carried out in NVT ensemble. The force field was ReaxFF in MS (Materials Studio) software, equilibration time was 1 ps, production time was 200 ps, time step was 0.1 fs, and frame output every 100 steps.

## 2.2. Simulation Results

2.2.1. The Mechanism of Pyrolysis Process

## a. Pyrolysis mechanism of balsa wood

After repeated simulations, it was found that glycosidic bonds broke first at the beginning of the reaction, because the dissociation energy of the glycosidic bonds was the lowest. Then the main chain was broken and the DP decreased, as shown in Figure 3. This was consistent with the conclusion in [24] that the DP of the insulation paper decreased rapidly during lasting high temperature experiments. At the same time, the number of hydrogen atoms and hydroxyls dropped, and some single bonds turned to double bonds and triple bonds. These highly active free radicals (H<sup>-</sup>, OH<sup>-</sup>) combined to make water or abstracted other hydrogen atoms and hydroxyls from the main chain, which promoted its decomposition. Then the D-glucose rings were broken. The oxygen-containing bridging -O-C- bond in the glucose ring usually broke prior to other C–C bonds, and formed an aldehyde group or a carbonyl group, as shown in Figure 4. As the reaction progressed, some C–C bonds gradually broke and low-carbon molecules formed. Hydrogen atoms combine with each other to generate hydrogen (H<sub>2</sub>), then the main chain broke up and some small molecules were formed.



Figure 3. The glycosidic bond break at the beginning of the reaction.



Figure 4. The pyranoid rings break.

## b. Pyrolysis mechanism of PVC

As for PVC degradation process, the Cl atom substituents were the most unstable part and broke off first from the main chain, as shown in Figure 5. The active chlorine free radicals abstracted H atoms from the PVC chain, and formed HCl. The adjacent two C atoms, which have lost Cl atoms and H atoms, easily generate double bonds or triple bonds, or the interphase C atoms connect to form a ring, as shown in Figure 6. As the reaction progresses, the C–C bonds broke and low-carbon small

molecules were produced, and the DP decreased. However, these low-carbon molecules were not stable, and they were easily reconnected with the main chain. In addition, the tail carbon atoms sometimes connected with other PVC molecular chain, which made the DP increase, as shown in Figure 7. The C chains constantly broke and were restructured during the pyrolysis process, thus there was no regular pattern change in the DP of PVC.



Figure 5. The chlorine atoms falling off the main chain.



**Figure 6.** Formation of double bonds and ring structures: (**a**) the adjacent two C atoms generated double bond; and (**b**) the interphase C atoms connected to form a ring.



Figure 7. The tail carbon atoms connection with other PVC molecular chain and DP increase.

The residual DP (the ratio of the sum of maximum DP in single molecular split chains and the initial number of macromolecules) of PVC and cellulose was calculated, and the results are shown in Figure 8. As we can see, the DP of cellulose decreased rapidly and the DP of PVC fluctuated.



Figure 8. The DPs of cellulose and PVC at 4000 K.

a. Main gas products of balsa wood

The gas products of cellulose were very complex, including CO, CO<sub>2</sub>, H<sub>2</sub>O, H<sub>2</sub>, and a variety of low carbon compounds. This was consistent with the gas chromatography results of cellulose pyrolysis proposed by Luo et al. in [24].

## 1. H<sub>2</sub>O

 $H_2O$  was the main product in cellulose pyrolysis. The hydrogen atoms and hydroxyls in cellulose molecules were active, and were likely to break off the main chain. These free hydrogen and hydroxyl radicals could easily combine to form water molecules by the influence of hydrogen bonds, as shown in Figure 9. The simulation results showed that the water was not stable and was further involved in the generation of other products during the pyrolysis reaction, resulting in the water content decreasing, but new  $H_2O$  molecules were generated, thus the increase of water molecules showed a fluctuting trend.



**Figure 9.** The generation process of  $H_2O$ : (**a**) hydroxyl and hydrogen radicals break from carbon chain; and (**b**) formation of  $H_2O$  from dropped hydroxyl and hydrogen.

## 2. H<sub>2</sub>

As the reactions progresses, more and more hydrogen atoms are removed from the main chain at high temperature. Some of these highly reactive hydrogen radicals combined with hydroxyl radicals to give water, while some of them combined with each other to generate hydrogen, the others abstracted hydrogen atoms from other molecules to generate hydrogen and promote the pyrolysis.

## 3. CO<sub>2</sub>

After the pyranoid ring broke, as shown in Figure 10, the C1 atom connecting with the oxygen atoms in pyranoid rings and the oxygen atoms in glucosidic bond easily fell off the main chain to form  $CO_2$  while it lost the hydrogen atom, as shown in Figure 11. In addition, the C7 atom with the oxygen atoms in pyranoid rings and a hydroxyl group could drop off the main chain and generate a formic acid molecule, and this would turn into  $CO_2$  by dehydrogenation. Because there was no oxygen in this simulation, which was different from the actual environment, the production of  $CO_2$  was lower than it should be. In fact, carbon burning will occur when lightning strikes the blades, and a larger amount of  $CO_2$  is produced.

## 4. CO

In the oxygen-free simulation environment, CO was one of the most common products in cellulose pyrolysis. Formic acid molecules easily lose the hydrogen and hydroxyl group to produce CO. The other groups such as aldehyde groups, carbonyl groups and the carbon atoms with hydroxyl groups were likely to produce CO. In addition, the existing CO<sub>2</sub> could be reduced to CO under the strong reducing action of hydrogen radicals.



Figure 10. The break pathway of pyranoid rings.



Figure 11. The generation process of CO<sub>2</sub>: (a) C–C bond break; and (b) CO<sub>2</sub> generation.

## 5. C<sub>2</sub>H<sub>2</sub>

Acetylene was another main product in cellulose pyrolysis. After the hydrogen atoms and hydroxyl groups fell off, the saturation of main chain and existing small molecules was very low, and many single bonds turned into double or triple bonds. Some double carbon intermediate products such as ethynol (HC $\equiv$ COH), unsaturated C<sub>2</sub> (C $\equiv$ C), and unstable ethylene glycol ( $_{HO/}^{H\setminus}C = C_{\backslash H}^{OH}$ ) could change into C<sub>2</sub>H<sub>2</sub> through the replacement of hydroxyls by H atoms (as shown in Figure 12), hydrogen absorption, or dehydroxylation.



**Figure 12.** The generation of  $C_2H_2$ : (**a**) unsaturated low-carbon hydrocarbon compounds capturing an H atom forming  $H_2O$ ; and (**b**)  $C_2H_2$  formation.

b. Main gas products of PVC

The main pyrolysis gas product of PVC was HCl,  $H_2$  and  $C_2H_2$ . There were also a few olefins and chlorohydrocarbons.

## 1. HCl

HCl was the main gaseous product in PVC pyrolysis, because the chlorine atoms in PVC are unstable and are easily removed from the main chain. The active chlorine radicals promoted the removal of H atoms from the PVC chain, and formed HCl as shown in Figure 13.



**Figure 13.** The generation of HCl: (**a**) Cl atoms dropped off the main chain; and (**b**) Cl radicals captured H atoms and formed HCl.

## 2. C<sub>2</sub>H<sub>4</sub>

Ethylene was mostly derived from the head or tail two carbon atoms falling off the long chain. There were also some ethylene and acetylenes that transformed into each other. The number of ethylenes in the earlier period was higher than in the later period, because many Cl atoms and H atoms were abstracted from the main chain, and the saturation level of the chain was low, thus the triple bond was more stable than double bond and some  $C_2H_4$  changed to  $C_2H_2$  or were added to main chain, leading to the slight decrease of  $C_2H_4$ , as shown in Figure 14.



**Figure 14.** The decrease of  $C_2H_2$ : (**a**) a  $C_2H_4$  and a  $C_2H_2$ ; (**b**)  $C_2H_4$  lost two H atoms and were changed into  $C_2H_2$ ; and (**c**)  $C_2H_4$  and  $C_2H_2$  lost one H atom and combined together.

## 3. $C_2H_2$

The simulation results showed that the number of  $C_2H_2$  molecules was nearly the same as that  $H_2$  ones at 4000 °C. The saturation of the PVC molecule was reduced after dechlorination and dehydrogenation, and double or triple bonds or ring structures were formed. As the reaction progressed, some C–C bonds broke and generated low carbon molecules, then the small molecules such as  $C_2H_4$  were reduced to  $C_2H_2$  and  $H_2$  as shown in Figure 15, or unstable intermediates  $C_2$  obtained two hydrogen atoms to produce  $C_2H_2$ , but  $C_2H_2$  and other low carbon molecules would also reconnect with the carbon chain, leading to an increase of DP, so the increase of  $C_2H_2$  fluctuated.



Figure 15. The generation of C<sub>2</sub>H<sub>2</sub>: (a) C<sub>2</sub>H<sub>4</sub> lost H atoms; and (b) C<sub>2</sub>H<sub>2</sub> was generated.

#### 4. H<sub>2</sub>

As the reaction progressed some C-H bonds broke at high temperature. These hydrogen radicals that were removed from the main chain were active and combined with each other to form  $H_2$  as shown in Figure 16, or abstracted H atoms from carbon chains or other small molecules to form hydrogen.



Figure 16. The generation of  $H_2$ : (a) uncombined H atoms; and (b) two H atoms combined to form  $H_2$ .

#### 2.2.3. Quantitative Comparison of the Gas Products of Cellulose and PVC

The expansion of the gas products at high temperature was an important material damage factor. In order to compare the amount of gas products of balsa wood and PVC, two models with the same volume of cellulose and PVC were set up in this paper. One cellulose molecule with a DP of 16 and nine PVC molecules with a DP of 4 were added in the two periodic cells respectively. The pyrolysis reaction was carried out at different temperatures to analyze the temperature influence on the two materials. The CO,  $CO_2$ ,  $H_2$ , HCl, other inorganic small molecules, low carbon hydrocarbons with less than five carbon atoms and the CHO compounds with only one carbon atom were considered as gas molecules in the simulation environment. The number of gas molecules produced by pyrolysis of cellulose and PVC at 4000 K and 2000 K are shown in Figure 17a,b, respectively.

As we can see from Figure 17, the gas molecules of cellulose were much more than those of PVC at high temperature, but the decomposition temperature of PVC was lower than that of cellulose, and the PVC generated gas and degraded earlier than cellulose when the temperature was not very high. The DP of cellulose decreased sharply at high temperature and generated a lot of low-carbon small molecules, in addition, dehydration and carbonization could also occur easily in cellulose and then the carbon combustion with the oxygen could occur in the actual environment, leading to more gas products. The DP of PVC fluctuated. On the one hand the long chains could break into low-carbon small molecules, which decreased the DP, while on the other hand the main chains or small molecules could connect with other chains, which increased the DP and decreased the gas products. Thus the gas products of cellulose were more than those of PVC. In addition, the breakage of Cl–C bonds in PVC needs more energy than the breakage of glycosidic bonds and pyranoid rings in cellulose,

so the Cl atoms came off the PVC earlier and the Cl radicals could easily abstract H atoms from PVC molecules and form HCl. As for cellulose, the glycosidic bonds and pyranoid rings broke first, and then the C–C bonds and C–O bonds broke to generate small gas molecules. This process needed more energy than PVC, thus the PVC generated gas molecules earlier than cellulose at 2000 K. But at 4000 K, both PVC and cellulose could get enough energy and generated gas quickly.



**Figure 17.** The number of gas molecules produced by cellulose and PVC: (**a**) Gas molecules number of balsa wood and PVC at 4000 K; and (**b**) Gas molecules number of balsa wood and PVC at 2000 K.

#### 3. Impact Current Experiments

## 3.1. Experimental Methods

The PVC and balsa wood of wind turbine blades were cut into  $15 \text{ cm} \times 10 \text{ cm} \times 2 \text{ cm}$  cuboids. In order to simulate the internal arc damage of material, two pieces of cuboid material were stacked together, and a nickel-chromium wire (d = 0.1 mm) was put between the two pieces of material. Then the specimen was fixed by insulating tape. One side of the nickel-chromium wire was connected to the high-voltage port of an impulse current generator and the other side of the wire was connected to the low-voltage port. When the wire was melted, the high temperature was used to simulate the thermal effect of the lightning arc. A diagram is shown in Figure 18.

Then the output current was set to an impact lightning current and the peak value was set to 1.45, 6.28, 12.5 and 21 kA, respectively. Then the impact currents with different peak values were added to the nickel-chromium wire to test the damage current of the two materials and observe their damage characteristics. The morphological damage features of the two materials were observed by scanning electron microscope (SEM) and the residual strength of the two materials was tested by a plastic pendulum bob shock testing machine.



Figure 18. The specimen diagrammatic sketch.

### 3.2. Experimental Results

## 3.2.1. Damage Morphology of the Two Materials

The two pieces of specimen were unfolded and the damage condition of the two materials is shown in Table 1. As we can see, there are carbonization traces along the nickel-chromium wire on the two pieces of material. The higher the peak current is, the bigger the carbonization areas are. There are obvious mechanical damages in both materials but the damage level is different. The upper layer of PVC was fractured when the peak current rose to 6.28 kA, and the two layers were both broken when the peak current rose to 12.56 kA. However, the upper layer of balsa wood was not broken until the peak current rose to 21 kA. Thus the damage current of PVC is lower than that of balsa wood.

The damage morphological features observed by SEM (magnification was 200 times) are shown in Figure 19. From the damage morphology we can see that the damage to PVC and balsa wood is different. The balsa wood damage showed itself as fractured fibers and missing material, and the PVC damage was mainly pore expansion. That was consistent with the simulation results: the pyrolysis results of cellulose consisted of main chain breakages, DP decrease and gas generation, which caused the fiber breakage and material defects.; the PVC chain broke and recombined in pyrolysis process and there was no obvious reduction in DP, so there was nearly no break in PVC damage, but PVC were softened locally under the effect of arc high temperature because the glass transition temperature of PVC was low, and the large amount of HCl and other gases produced in pyrolysis process could expand the gaps in the softened PVC. The experiment results were consistent with the simulation results.



Table 1. The damage conditions of PVC and balsa wood.

**Figure 19.** The morphological features of balsa wood and PVC: (**a**) undamaged balsa wood; (**b**) damaged balsa wood (21 kA); (**c**) undamaged PVC; and (**d**) damaged PVC (12.56 kA).

## 3.2.2. Damage Degree of the Two Materials

The sizes of the damage areas in the two materials were measured. The width size along the surface and the depth size of the two materials are shown in Tables 2 and 3, respectively. As we can see, the damage width was larger than the depth in balsa wood but the size of width and depth in PVC was not regular. The impact residual strength of the two materials is shown in Figure 20. It was found that the impact residual strength of PVC and balsa wood decreased with the increase of peak current, and the fall in PVC was faster. In addition, PVC was easier to fracture along the depth direction than balsa wood because arc heat in PVC spread non-directionally, but in balsa wood it spread along the surface direction.

Peak Value of Current	1.45 kA	6.28 kA	12.56 kA	21 kA
Width size (cm)	0.4	0.7	3	4.5
Depth size (cm)	0.1	0.2	2	2

**Table 2.** Damage width and depth of balsa wood.



Table 3. Damage width and depth of PVC.

Figure 20. Curve of residual strength vs current peak value.

## 4. The Comparison of Balsa Wood and PVC

The damage characteristics of balsa wood and PVC were compared.

- 1. The pyrolysis temperature of PVC was found lower than that of balsa wood. According to the pyrolysis simulation of the two materials at different temperatures, the release of HCl in PVC occurred earlier than glycosidic bond breaks in balsa wood at the same temperature, so that the heat resistance of balsa wood was better than that of PVC. The impact experiments also showed that the PVC was damaged at a lower current than balsa wood. In addition, PVC softened easily at high temperature because its glass transition temperature is low (78–81 °C), and the ultraviolet light and oxygen could also cause photooxidation of PVC, causing the flexibility of PVC to decrease, thus in the strong light and high temperature areas balsa wood resulted better than PVC as blade material.
- 2. The rigidity of cellulose decreased greatly during pyrolysis. The cellulose has stronger rigidity compared with PVC. Firstly the molecular polarity of cellulose made the interaction between the molecular chains stronger; secondly the hexagonal pyranoid rings in the molecule made

the chain rotation difficult; thirdly there were a lot of hydrogen bonds in the molecules or between molecules, especially intramolecular hydrogen bonds, making the glycosidic bonds unable to rotate, so the rigidity of balsa wood is greatly increased. However, it could be seen from the pyrolysis of cellulose that the glycosidic bonds broke during the pyrolysis process, the DP decreased sharply, the pyranoid ring structure was broken, and the intramolecular hydrogen bonds were changed, as shown in Figure 21, so the molecular chain structure was destroyed, and thus the rigidity of the cellulose was greatly reduced.

- 3. The decomposition of cellulose was mainly due to the breakage of the chains, the decrease of DP, and formation of a lot of gaseous products, leading to macroscopic fiber fractures and missing materials. The decomposition of PVC was mainly shown in terms of release of HCl gas, and other small gas molecules would be generated in further reaction, and the molecular chains broke and reconnected constantly. Considering its low softening temperature, the damage of PVC was mainly shown as pore extension on a macroscopic level.
- 4. The main air products of balsa wood in the simulation were CO, H<sub>2</sub>O, H<sub>2</sub> and C<sub>2</sub>H<sub>2</sub>. Those of PVC were HCl, H<sub>2</sub>, and C<sub>2</sub>H<sub>2</sub>. The gas product expansion accelerated the fiber fracture in balsa wood and the pore extension in PVC. According to the simulation results, the gas products of balsa wood were much more plentiful than those of PVC, so the material damage caused by gas products was more serious in balsa wood. In addition, because the cellulose in the balsa wood can generate hydrogen bonds with the water molecules in the surrounding environment, the moisture content of balsa wood is much higher than that of PVC. On the one hand, the water molecules could promote the pyrolysis of the cellulose; on the other hand, the combined water would evaporate at high temperature, which could also exacerbate balsa wood damage, so PVC was better than balsa wood as a turbine blade material in humid areas (such as those where offshore wind turbines are installed).



**Figure 21.** The hydrogen bonds in cellulose: (**a**) the hydrogen bonds before pyrolysis; and (**b**) the hydrogen bonds were destroyed during pyrolysis.

## 5. Conclusions

Lightning arcs can cause serious mechanical damage to both balsa wood and PVC. However the damage characteristics in PVC and cellulose were different. In PVC the Cl atoms were active and easily captured H atoms and formed HCl. The first stage of PVC decomposition was rapid and the reaction temperature was lower than in cellulose, so that the gas was produced earlier in PVC than in cellulose at 2000 K. In cellulose, the dissociation energy of glycosidic bonds is low and they broke first. Both PVC and cellulose would produce a lot of gas products during the reaction, which could expand and cause further damage to the two materials at high temperature, and the gas amount was higher in cellulose than that produced by the same volume of PVC. In addition, the DP of cellulose decreased sharply while the DP of PVC decreased and increased irregularly during degradation.

The impact current experiment results allowed to test the simulation results. The damage characteristics of PVC and balsa wood were different: the mechanical damage of PVC was mainly shown as pore expansion because the gas products expanded and the glass transition temperature of PVC was low; the damage on cellulose was mainly shown as fiber breakage and missing material, because the DP decreased sharply during the pyrolysis process and a lot of low carbon gas products were generated. The mechanical strength of cellulose is strongly reduced. The damage current of PVC was lower than that of balsa wood and the damage of PVC was also more serious than that of balsa wood at the same impact current, thus the lightning tolerance level of balsa wood was higher than that of PVC. However, the water content in balsa wood is higher than that in PVC, and the water expands at high temperature would increase the damage of balsa wood. Thus as much of the internal moisture in balsa wood should be removed as possible. What's more, in humid areas, especially in the case of offshore wind farms, PVC is better than balsa wood as a blade sandwich material.

**Acknowledgments:** This work was supported by the National Science Foundation of China under Grant Nos. 51677110 and 51420105011, and State Key Laboratory of Alternate Electrical Power System with Renewable Energy Sources (LAPS16018).

**Author Contributions:** Li Zhang and Liang Zou conceived and designed the impact current experiments; Li Zhang performed the experiments; Li Zhang and Liyang Jiang conceived and designed the molecular simulation; Liyang Jiang performed the simulation; Li Zhang and Liyang Jiang analyzed the data; Tong Zhao contributed materials and analysis tools; Liyang Jiang wrote the paper.

**Conflicts of Interest:** The authors declare no conflict of interest.

## References

- Rachidi, F.; Rubinstein, M.; Montanya, J.; Bermudez, J.L.; Sola, R.R.; Sola, G.; Korovkin, N. A Review of Current Issues in Lightning Protection of New Generation. *IEEE Trans. Ind. Electron.* 2008, 55, 2489–2496. [CrossRef]
- 2. Cotton, I.; Jenkins, N.; Pandiaraj, K. Lightning protection for wind turbine blades and bearings. *Wind. Energy* **2001**, *4*, 23–37. [CrossRef]
- Piwko, R.; Miller, N.; Sanchez-Gasca, J.; Yuan, X.; Dai, R.; Lyons, J. Integrating large wind farms into weak power grids with long transmission lines. In Proceedings of the CES/IEEE 5th International Power Electronics and Motion Control Conference (IPEMC 2006), Shanghai, China, 14–16 August 2006; IEEE: Piscataway, NJ, USA, 2006; pp. 1–7.
- 4. Tsai, K.C.; Pan, C.T.; Cooperman, A.; Johnson, S.; van Dam, C. An Innovative Design of a Microtab Deployment Mechanism for Active Aerodynamic Load Control. *Energies* **2015**, *8*, 5885–5897. [CrossRef]
- 5. Fernandez-Gamiz, U.; Zulueta, E.; Boyano, A.; Ramos-Hernanz, J.A.; Lopez-Guede, J.M. Microtab Design and Implementation on a 5 MW Wind Turbine. *Appl. Sci.* **2017**, *7*, 536. [CrossRef]
- 6. Toshio, O.; Yoshiyasu, H.; Akinori, Y. Coupled thermal–electrical analysis for carbon fiber epoxy composites exposed. *Compos. Part A* **2010**, *41*, 973–981.
- Vasa, N. J.; Naka, T.; Yokoyama, S.; Wada, A.; Asakawa, A.; Arinaga, S. Experimental Study on Lightning Attachment Manner considering Various Types of Lightning Protection Measures on Wind Tuine Blades. In Proceedings of the International Conference on Lightning Protection, Kanazawa, Japan, 17–21 September 2006; pp. 1483–1487.
- 8. Feraboli, P.; Miller, M. Damage resistance and tolerance of carbon epoxy composite coupons subjected. *Compos. Part A* **2009**, *40*, 954–967. [CrossRef]
- 9. Kithil, R. *Case Study of Lightning Damage to Wind Turbine Blade;* National Lightning Safety Institute: Louisville, CO, USA, 2008.
- 10. Adri, C.T.; Siddharth, D.; Francois, L.; William, A.G. ReaxFF: A reactive force field for hydrocarbons. *J. Phys. Chem. A* **2001**, *105*, 9396–9409.
- 11. Kimberly, C.; Adri, C.T.; William, A.G. ReaxFF Reactive Force Field for Molecular Dynamics Simulations of Hydrocarbon Oxidation. *J. Phys. Chem. A* **2008**, *112*, 1040–1053.
- 12. Adri, C.T.; Yehuda, Z.; Faina, D.; Ronnie, K. Atomistic-Scale Simulations of the Initial Chemical Events in the Thermal Initiation of Triacetonetriperoxide. *J. Am. Chem. Soc.* **2005**, *127*, 11053–11062.

- Ken-ichi, N.; Rajiv, K.K.; Aiichiro, N.; Priya, V.; van Duin, A.C.T.; Goddard, W.A., III. Dynamic Transition in the Structure of an Energetic Crystal during Chemical Reactions at Shock Front Prior to Detonation. *Phys. Rev. Lett.* 2007, *99*, 148303. [CrossRef]
- 14. Akira, T.; Akihisa, I. Calculations of Mixing Enthalpy and Mismatch Entropy for Ternary Amorphous Alloys. *Mater. Trans. JIM* **2007**, *41*, 1372–1378.
- 15. Miller, J.A.; Pilling, M.J.; Troe, J. Unraveling combustion mechanisms through a quantitative understanding of elementary reactions. *Proc. Combust. Inst.* **2005**, *30*, 43–88. [CrossRef]
- Goddard, W.A., III; Mueller, J.E.; Chenoweth, K.; van Duin, A.C.T. ReaxFF Monte Carlo reactive dynamics: Application to resolving the partial occupations of the M1 phase of the MoVNbTeO catalyst. *Catal. Today* 2010, 157, 71–76. [CrossRef]
- Goddard, W.A.; Adri, C.T.; Chenoweth, K.; van Duin, A.; Chenoweth, K.; Cheng, M.J.; Pudar, S.; Oxgaard, J.; Merinov, B.; Jang, Y.H.; et al. Development of the ReaxFF reactive force field for mechanistic studies of catalytic selective oxidation processes on BiMoOx. *Top. Catal.* 2006, *38*, 93–103. [CrossRef]
- Chenoweth, K.; Adri, C.T.; Goddard, W.A. The ReaxFF Monte Carlo Reactive Dynamics Method for Predicting Atomistic Structures of Disordered Ceramics: Application to the Mo3VOx Catalyst. *Angew. Chem. Int. Ed.* 2009, 121, 7766–7770. [CrossRef]
- Nielson, K.D.; van Duin, A.C.T.; Oxgaard, J.; Deng, W.Q.; Goddard, W.A. Development of the ReaxFF Reactive Force Field for Describing Transition Metal Catalyzed Reactions, with Application to the Initial Stages of the Catalytic Formation of Carbon Nanotubes. *J. Phys. Chem. A* 2005, 109, 493–499. [CrossRef] [PubMed]
- Zhong, Y.; Jing, X.; Wang, S.; Jia, Q.X. Behavior investigation of phenolic hydroxyl groups during the pyrolysis of cured phenolic resin via molecular dynamics simulation. *Polym. Degrad. Stab.* 2016, 125, 97–104. [CrossRef]
- 21. Zeng, F.; Peng, C.; Liu, Y.; Qu, J. Reactive Molecular Dynamics Simulations on the Disintegration of PVDF, FP-POSS, and Their Composite during Atomic Oxygen Impact. *J. Phys. Chem. A* 2015, *119*, 8359–8368. [CrossRef] [PubMed]
- 22. Li, H.; Ren, D.; Cheng, X. The theoretical investigation of the β-crystobalite structure under the effect of electric field. *Comput. Mater. Sci.* **2015**, *96*, 306–311. [CrossRef]
- 23. Diao, Z.; Zhao, Y.; Chen, B.; Duan, C.; Song, S. ReaxFF reactive force field for molecular dynamics simulations of epoxy resin thermal decomposition with model compound. *J. Anal. Appl. Pyrolysis* **2013**, *104*, 618–624. [CrossRef]
- 24. Luo, Z.; Wang, S.; Liao, Y.; Cen, K. Mechanism Study of Cellulose Rapid Pyrolysis. *Ind. Eng. Chem. Res.* **2004**, *43*, 5605–5610. [CrossRef]



© 2017 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by/4.0/).