

# Mechanical and molecular studies of biocomposites filled with oil palm empty fruit bunches microfibers

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**Abstract.** The present work aims to investigate mechanical and molecular characteristics of acrylonitrile butadiene styrene (ABS) composites filled with oil palm empty fruit bunches (OPEFB) microfibers. OPEFB microfibers were produced using mechanical milling. Composite granules were fabricated using single screw extruder. These composites were then used for fabricating helmet according to the Indonesian National Standard (SNI). Mechanical testing confirms that the helmet produced using this biocomposites are suitable to the SNI. Molecular interaction between matrix with OPEFB can be described using orbital hybridization theory. In general, this study has successfully investigated mechanical and molecular properties of the biocomposites.

## 1. Introduction

Indonesia becomes the biggest producer oil palm in the world. It is estimated that Indonesia contributes 48% of the total volume of palm oil production. In 2014, its production reaches 31.5 million tons, where the quantity has stably increased for the last 20 years with 11% every year. In 2020, Indonesia's Crude Palm Oil (CPO) is estimated to reach 40 million ton. Every ton of the processed oil palm fresh fruit bunches (OPFFB) produces about 50% of the total waste, while the processed oil palm empty fruit bunches (OPEFB) produces about 23% of the total waste. These wastes became a serious problem since they were directly discharged to the environment. Utilization of these materials for various purposes is an interesting study to be explored [1-4]. Moreover, several works have been carried out to investigate their physical, chemical, and biological properties [5-9].

Furthermore, the present work aims to investigate mechanical and molecular characteristics of acrylonitrile butadiene styrene (ABS) composites filled with OPEFB microfibers. These knowledges are essential for comprehensive evaluation their composite properties in terms of macroscopic and microscopic scales.

OPEFB are widely known to contain a lot of fibers and celluloses that are potential to be explored as filler for producing biocomposite materials [2]. OPEFB's fiber is able to bind with ABS ( $(C_8H_8 \cdot C_4H_6 \cdot C_3H_3N)_x$ ) polymer through compatibilizer in a composite structure. Binding between OPEFB fiber and ABS polymer can be explained by the molecular orbital theory. The molecular orbital theory stated that the binding molecules occurred was due to the hybridisation of the orbitals for each molecules [10, 11]. When OPEFB fiber molecules placed near with the ABS molecules, the wave functions of each molecule are superpositioned linearly, forming hybrid binding having the hybrid



energy levels characteristics, which principally can be found by solving the multiatomic Schrodinger equation.

## 2. Experimental

### 2.1. Materials

In this work, OPEFB were obtained from PT Perkebunan Nusantara VIII Cikasungka, Bogor. Recycled/virgin ABS was obtained from PT MUB Jaya Cibinong. In addition, additives used for manufacturing composites granules are antioxidants primer (butylated hydroxytoluene) from Mumbai, India, scavenger acid (calcium stearate) from Mumbai, India, and compatibilizer (maleic anhydride) from Darmstadt, Germany.

### 2.2. Filler production

OPEFB were washed to be cleaned of impurities and enumerations and then cut into chip size. Then, they were dried at 100 °C for 8 hours to reduce their water content. OPEFB were milled using milling machine at a speed of 25.000 rpm for 5 min. The results of the first milling were sieved to 20 mesh sieve in order to separate the large fibers and tiny fibers. Large fibers (retained 20 mesh) were then milled until their size were able to pass through the sieve. For the fibers passing 20 mesh were continued with a 60-mesh sieve and followed by 100 mesh sieve. While the fiber cannot pass through the sieve are reprocessed as aforementioned treatments. In the present study, fibers passing a 100 mesh, which are about 150  $\mu\text{m}$  in size, were used for biocomposite fillers.

### 2.3. Manufacture of composite granules

Biocomposite granules were fabricated by combining filler, recycled/virgin polymer (matrix) with additives using industrial scale machine. The biocomposites were produced by extrusion using single-screw extruder machine (Model HXSJ-125/125, Kai Xin, China) with 15 wt% filler, 81.7 wt% recycled ABS polymer, and 1 wt% primary antioxidant (China), 0.3 wt% acid scavenger (Germany), and 2 wt% coupling agent (Germany). In the barrel, the samples were blended with gradient temperatures of 195, 215, 220, 220, 220, 225, 225, and 225 °C. The composition of each material is then listed in Table 1.

**Table 1.** Composition of biocomposites.

Code	OPEFB	Polymer	Material additive
SN-1	Microfiber 15%	Recycled ABS	Antioxidan 1% Acid Scavenger 0.3% Maleic Acid 2%
SN-2	Microfiber 15%	Virgin ABS	Antioxidan 1% Acid Scavenger 0.3% Maleic Acid 2%

### 2.4. Test

ABB FTIR MB3000 model equipped with MB3000 software, Québec, Canada were employed for FTIR analysis. In this investigation, wave numbers from 450 to 4000  $\text{cm}^{-1}$  at a resolution of 4  $\text{cm}^{-1}$  was used. Pellets were produced by mixing biocomposites and KBr with a ratio of 1:100 using a hydraulic press at a pressure of 10 tons. The pellets were then placed in the FTIR holder and FTIR spectra were recorded. Mechanical properties of the helmet produced using this biocomposite materials were tested according to the Indonesian National Standard (SNI).

### 2.5. Molecular orbital theory

Molecular orbital theory states that the bonding molecules are due to hybridization of their orbital. It is obtained from linear superposition of orbital wave function. Wave function  $\psi$  can be developed from linear combination of basis function  $\phi_i$  as follows:

$$\psi = \sum_i^n c_i \phi_i \quad (1)$$

where  $c_i$  is optimum using variation principle as a result its energy is minimum. Function  $\phi_i$  is defined as orbital molecular.

The strength of the bond between the two molecular orbitals is affected by its molecular symmetry and type of bonding orbitals hybridize. Two types of bonding are  $\sigma$  and  $\pi$  bonds. In the bond  $\sigma$ , its line symmetrical electron density is concentrated along the line connecting the two atoms. For instance, Figure 1 shows the formation of the  $\sigma$  bond between two molecules. Moreover, the  $\pi$  bond is a bond where its superposition area is above and below the internuclear axis (see Figure 2).

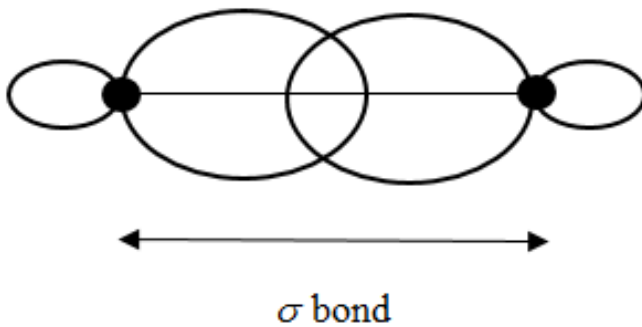


Figure 1.  $\sigma$  bond

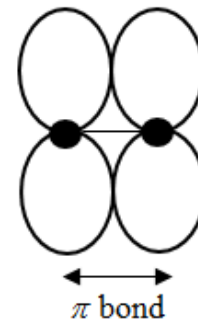


Figure 2.  $\pi$  bond

The number of bond that can be formed is crucially affected by the number of the valence electron at level bonding and antibonding and then can be estimated using the following equation:

$$N_{bond} = \frac{1}{2}(n_{eb} - n_{eab}) \quad (2)$$

where  $n_{eb}$  is the number of valence electron at bonding level and  $n_{eab}$  is the number of valence electron at antibonding level.

## 3. Results and Discussions

### 3.1 Biocomposite production

OPEFB fibers, recycled polymer and additives were prepared according to Table 1. Then the materials inserted into the mixing machine. Mixing was carried out to bind the material. The use of additives in this research is useful to maintain condition of the plastic/polymer used. In addition, antioxidant additive serves to prevent the oxidation reaction by oxygen that can cause degradation of the polymer. Acid scavenger acts to neutralize the acid formed during the extrusion process so that the polymer chains are not degraded. Moreover, the coupling agent serves to increase the degree of dispersion, where the coupling agent acts as the interface that affect the interfacial adhesion and interfacial tension. The Interfacial adhesion increases while the interfacial tension decreases with addition of the coupling agent.

The extrusion is a polymer material process by pressing the polymer through a mold cavity arranged magnitude. On the machine, there is a screw extruder that rotates so that the material can lead to the extrusion machine parts ranging from the feed zone and melting zone to the melt-pumping zone. In this work, single screw extruder that only has one screw is placed in the barrel. The material which is shaped like an elongated "noodles", was pulled through the water for cooling and hardening. Inside this machine, the composites were cut into small shape as shown in Figure 3.



**Figure 3.** Biocomposite granules

### 3.2 Mechanical properties

Composites granules were then used to produce a helmet using molding machine. Table 2 lists mechanical properties of the helmets. As previously mentioned, testing was conducted according to the SNI. The testing was carried out using three different temperatures. This study found that the impacts of the helmet at a temperature of  $-20\text{ }^{\circ}\text{C}$  are in the range of 81.3 to 121.7. In addition, their impacts at temperatures of 15 and  $50\text{ }^{\circ}\text{C}$  are in the ranges of 84.6 to 152.1 and 113.2 to 137.9, respectively. Moreover, this work confirmed that this helmet was suitable according to the SNI in terms of its impact and head injury criteria.

### 3.3 Molecular Analysis

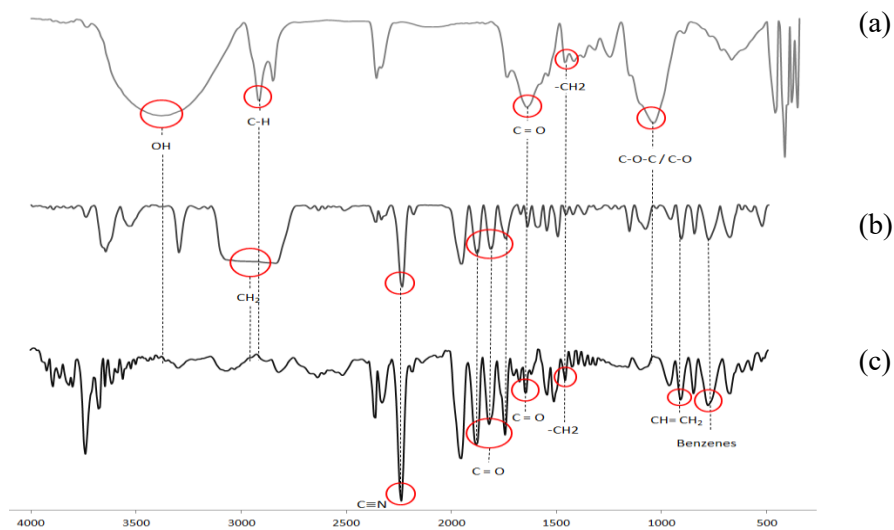
FTIR spectra of OPEFB (filler), recycled/virgin ABS (matrix), and biocomposites are depicted in Figures 4 and 5. FTIR spectra of biocomposites were dominated by the peaks of the matrix, which are  $2237\text{ cm}^{-1}$  ( $\text{N}\equiv\text{C}$ ) and  $1600\text{--}1900\text{ cm}^{-1}$  ( $\text{C}=\text{O}$ ) of the polymer ABS as well as in the range of  $670\text{--}1000\text{ cm}^{-1}$  ( $\text{CH}=\text{CH}_2$  benzene). In addition, the peak appearing at wave number  $2360\text{ cm}^{-1}$  and  $1627\text{ cm}^{-1}$  are derived from the filler. Their dominance peaks from recycled ABS are due to the composition of the biocomposite is generally recycled ABS. As previously mentioned that OPEFB are 15% of the total biocomposites.

Furthermore, bond formation between cellulose molecules and ABS can be explained by the theory of orbital hybridization. There are several bonds namely single, double, and triple bonds. This is influenced by the charging of valence electrons in the level of hybridization. For instance, the bond is called hybridization  $\text{sp}$  if it involves only  $s$  and  $p$  orbitals. The amount of the bond is determined by the difference between the number of the valence electrons in the antibonding and bonding level. Understanding the formation of bonds in complex molecules is necessary to understand the process of the formation of a hybrid bond in the molecule. For example, based on the calculation of molecular orbital theory, the energy levels of  $\text{C-O}$  can be seen in Figure 6.

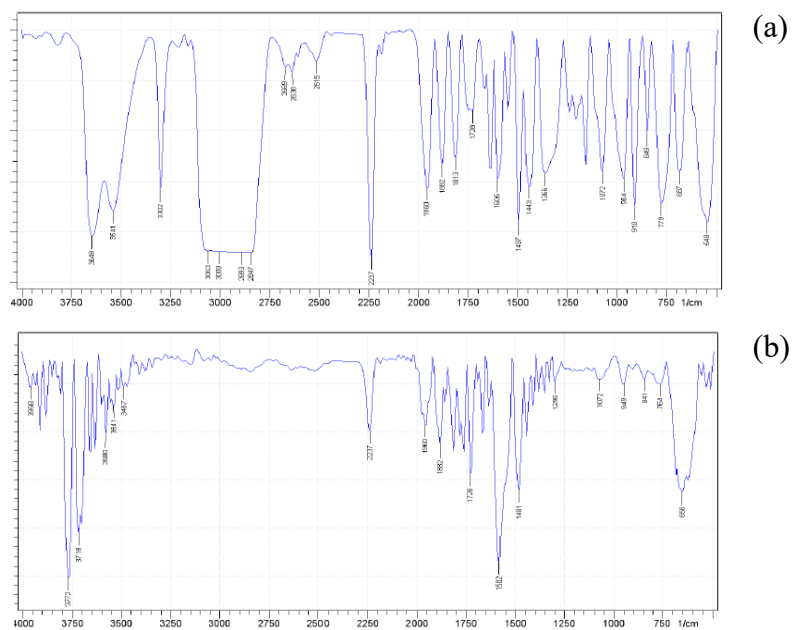
**Table 2.** Mechanical properties of the helmets.

Code	Temperature (°C)	Clash position	Paron type	The impact in units of gravity	Suitability of SNI	Head injury criteria	Suitability of SNI
SN1	-20	backside	flat paron-1	121.7	suitable	760	suitable
			flat paron -2	103.6	suitable	398	suitable
		on the top	hemispherikal paron	81.3	suitable	335	suitable
	15	backside	flat paron-1	145.0	suitable	1090	suitable
			flat paron-2	152.1	suitable	797	suitable
		on the top	hemispherikal paron	84.6	suitable	373	suitable
	50	backside	flat paron-1	137.9	suitable	799	suitable
			flat paron-2	113.2	suitable	433	suitable
		on the top	hemispherikal paron	127.4	suitable	453	suitable
SN2	-20	backside	flat paron-1	151.7	suitable	1141	suitable
			flat paron-2	133.6	suitable	662	suitable
		on the top	hemispherikal paron	86.1	suitable	334	suitable
	15	backside	flat paron-1	148.8	suitable	1090	suitable
			flat paron-2	153.6	suitable	791	suitable
		on the top	hemispherikal paron	93.7	suitable	415	suitable
	50	backside	flat paron-1	130.3	suitable	980	suitable
			flat paron-2	122.2	suitable	587	suitable
		on the top	hemispherikal paron	101.7	suitable	411	suitable

Bonding C-O involves one  $\sigma$  bond and two  $\pi$  bond (Figure 7). It has a distance of 1.1 Å so consistent with a triple bond. In comparison, a single binding C-O has a distance of 1.43 Å and double bind C-O within Average 1.23 Å. In this study, FTIR spectrum of C-O is around 1000  $\text{cm}^{-1}$ . C-O bond was formed on the kind of p orbitals serve as bonding orbitals. From Figure 6, it can be seen that there are 4 valence electrons in the atom C, two in the 3p level and two at level s with a total molecular orbital of 4. In addition, for O, there are 6 valence electrons, 4 in 3p level and two at s lvel with total number of orbital level 4.

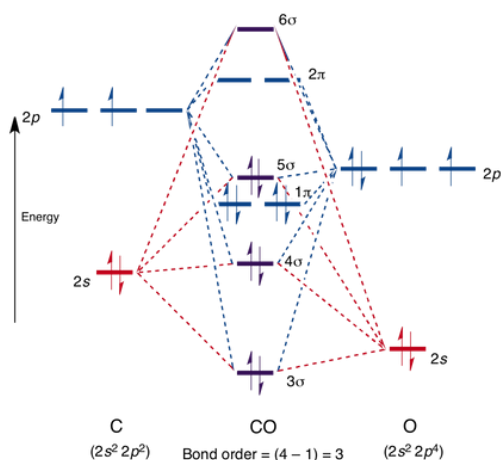


**Figure 4.** FTIR spectra of (a) OPEFB fiber, (b) recycled ABS, and (c) biocomposite (SN1)

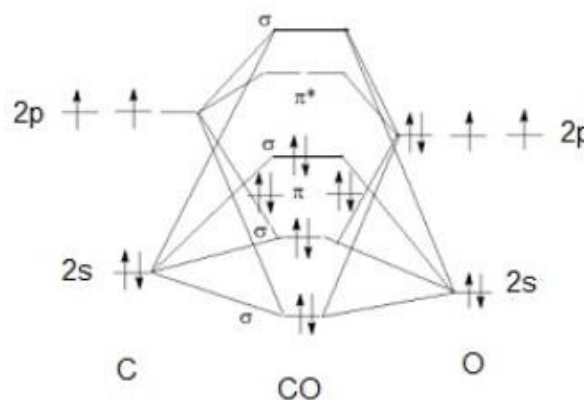


**Figure 5.** FTIR spectra of (a) virgin ABS and (b) biocomposite (SN2)

After hybridization level, the combined energy is  $4 + 4 = 8$ . Explanation of bond formation for more complex molecules is necessary information about the levels of the complete hybrid. The number of hybrid orbitals level ABS-OPEFB fiber is the summation of the quantities of each molecular orbital ABS and fiber TKKS. The type and amount of the bond that is formed depend on their valence electron.



**Figure 6.** Energy level diagram of C-O [12]



**Figure 7.** Molecular orbital of diagram of C-O [13]

#### 4. Conclusion

This study aims to investigate mechanical and molecular properties of acrylonitrile butadiene styrene composites filled with OPEFB microfibers. Mechanical properties of helmets are suitable according to the SNI. FTIR spectra confirmed the presence of functional groups from filler and matrix composite. Basically, the molecular interaction between the matrix with filler can be explained by the theory of the orbital hybridization. However, explanation bond formation for more complex molecules like this work needs information on levels of the complete hybrid.

#### Acknowledgement

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