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Molecular Dynamics Study for the Temperature & Moisture Effect on Mechanical Property and Thermal Stability of PMIA Insulation Paper

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This paper aims to study the temperature and moisture effect on the poly-m-phenylene isophthalamide (PMIA) mechanical property and thermal stability by adopting molecular dynamics method (MD). The study shows that as the temperature increases, the PMIA rigidity weakens, and the plasticity and ductility are increased; also, the mean square displacement (MSD) and gyration radius of PMIA increases with temperature increasing, and the chain motion of PMIA is intensified, i.e. thermal stability drops. As the moisture content increases, the PMIA rigidity weakens, and the plasticity and ductility are increased with the moisture content; compared with the situation in the lower water content (<2%) and higher water content (4% and 5%), the chain motion of complex model is more intensified, indicating that the PMIA thermal stability gradually decreases with the water content increasing.

1. Introduction

As one of the most important equipment, the reliable operation of power transformer safeguards the electrical power system. The insulation paper, mostly made of cellulose, has become one of the most significant industrial materials, owing to its rich reserves, reproductivity, and good electrical mechanical property. In the long-term operation, the internal oil-paper insulation of the transformer could be influenced by such factors as electric field, temperature field, moisture and acid, to cause the oil-paper insulation decomposing and aging; among these factors, the temperature and moisture are the key ones influencing the oil-paper insulation (Fofana et al., 2002).

All the properties of transformer are greatly related to the temperature. The relevant researches showed that every time the temperature increased 10 ℃, the insulation material performance would reduce one half (Lessard et al., 1996). Liao et al., (2011) Chongqing University, conducted lots of researches for the temperature effect on the oil-paper insulation property, finding that the temperature could reduce the rigidity of insulation paper, increase its plasticity, and also weaken the cellulosic stability. The temperature also had effects on the rate of oil-paper insulation moisture, furfural and oxygen, and the distribution of micro-molecule outcome in oil-paper insulation (Liao et al., 2017). The study of Chi et al. (2015) indicated that the temperature rise could lead to changes of electric field intensity of oil-paper insulation.

The oil-paper insulation constitutes the main insulation structure of oil-immersed power transformer. In long-term operation process for the transformer, the insulation oil may decompose and generate moisture, which can speed up the aging of insulation paper, and reduce its mechanical property, thermal stability and dielectric property. The research of the domestic and foreign scholars (Zhou et al., 2014; Liao et al., 2010; Żukowski et al., 2015) showed, the moisture had become the No.1 enemy for oil-paper insulation. In lower moisture content, the degradation rate of insulation paper was less influenced, while in higher moisture content, the degradation rate was increased (Liao et al., 2012). Emsley et al. made research, and found that the moisture content of insulation paper and its degradation rate had direct ratio relation: every time its water content increased 0.5%, the lifetime of insulation would reduce one half (Emsley and Stevens, 1994). The aging rate

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of insulation paper in the 1% moisture content was 10 times of that in 0.1% moisture content (Lundgaard et al., 2004).

As one new excellent type of high-strength and high-module material, the aramid fibre has been widely applied in the fields such as aerospace, military, electric communication and civil industry. PMIA fibre has good thermal stability, even in the high temperature environment of 220 ℃ for ten years; at 330 ℃, it wouldn't shrink or melt etc. (Villar-Rodil et al., 2001; Kong et al., 2013; Lin et al., 2016). Besides, PMIA also has sound property of fire resistance and electrical insulation. Therefore, in recent years, the PMIA has been applied in the oil-paper insulation system of the transformer more widely. To further study the influencing mechanism of temperature/water on PMIA performance has become one importance trend.

Now, most researches have been based on the macroscopical test methods, but few researches on the temperature and moisture effect on the PMIA micro-mechanism. For this, the molecular simulation technique could help to provide one reliable approach, adopting MD method to demonstrate the temperature and moisture effect on PMIA performance from the micro perspective. Hence, this paper adopts the material studio (MS) software to make dynamics analysis of PMIA fibre model, analysing the temperature and moisture effect on PMIA performance.

2. Model construction and calculation

2.1 Model construction

Considering that in long-term operation for the oil-immersed transformer, the moisture content in the insulation paper may increase to 5%, the PMIA-moisture complex model was constructed with moisture content 0%, 1%, 2%, 3%, 4%, and 5%; considering that the hot-spot temperature of local environment in transformer can reach 150 ℃, the temperature was set at 70 ℃, 90 ℃, 110 ℃, 130 ℃ and 150 ℃; then the simulation analysis was made to the PMIA fibre performance respectively (Zhu et al., 2015; Wang et al., 2013).

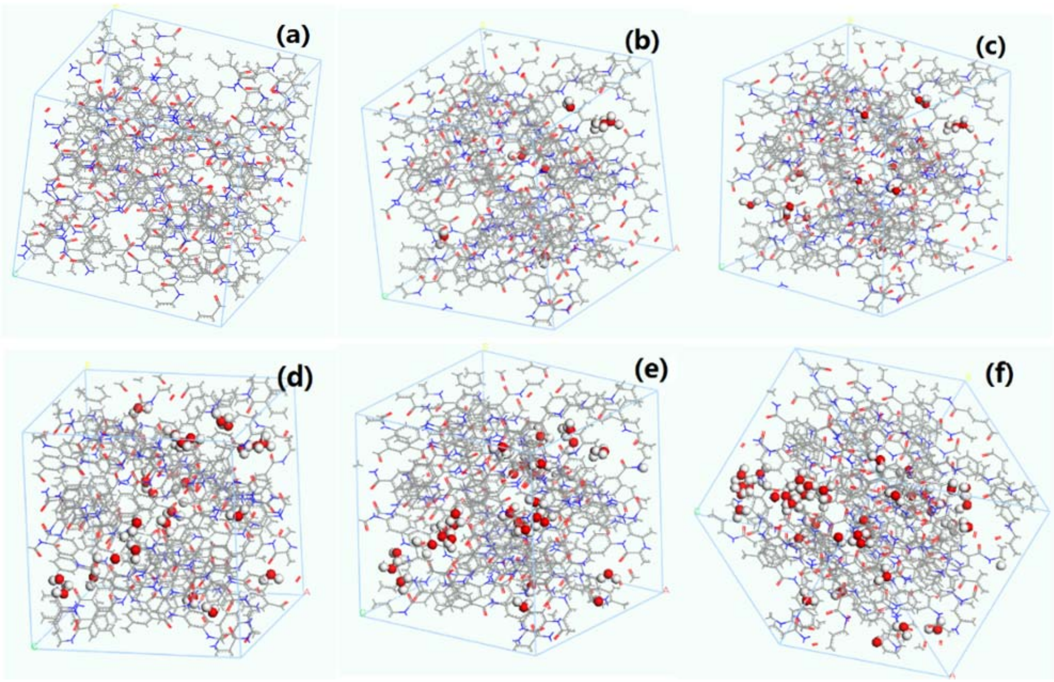

Figure 1: PMIA complex model in different moisture contents ((a)-(f) represent 0%-5%, respectively)

Firstly, apply the Visualizer model in the MS software package to construct the PMIA and water molecule model at 20 Degree of polymerization (DP), and then use the Amorphous Cell model to construct the different-moisture content complex model; to eliminate the boundary effect and stabilize the system density, the periodic boundary condition (PMC) and 1.4 g/cc (Tang et al., 2017) density was adopted. Refer to Figure 1(a)-(f) for the complex model in different moisture contents.

2.2 MD simulation calculation

Make energy minimization of the constructed complex model, set the iteration step for 5000, take system optimization in Forcite model, and then make annealing treatment at the annealing temperature 300-1000 K for the optimized complex model. Finally, the complex model of thermodynamic stability was obtained. Next, the MD simulation was made: firstly, conduct the 100ps dynamics simulation in the NVT ensemble, then change to NPT ensemble for 100ps dynamic simulation with the selected time 1fs step; select Compass force field, and Anderson temperature control method and Berendsen method for molecular dynamics simulation. Besides, use Maxwell distribution for initial speed distribution, Atom Based method for van der Waals force and Coulomb force, and set the Truncation radius as 0.95 nm (Zhang et al., 2012; Yin et al., 2006; Li et al., 2017).

3. Calculation result analysis

The aging of insulation paper can be divided into electrical aging and mechanical property aging. Generally, the aging of PMIA insulation property had little influence on the whole performance of the insulation paper, while the degradation of mechanical property was the main factor influencing the mechanical property of insulation paper. In theory, all the mechanical properties of solid material can be derived in the generalized Hooke Law matrix, with 6×6 elastic coefficient matrix. For the substance made of heterogeneous materials, it produces different elastic effect for all internal points; for the substance of homogeneous materials, under the relevant stress on the internal points, it is inevitable to have strains accordingly, vice versa. Due to the existence of strain energy, among the 36 elastic constants, even if it is an extreme Anisotropic elastomer, only with 21 elastic constants, the mechanical property can be described; 13 elastic constants are needed for the anisotropic elastomer with one symmetrical elastic surface; 9 needed for orthotropic elastomer; 5 needed for transverse isotropic elastomer.

3.1 Temperature effect on PMIA performance

3.1.1 Mechanical property

According to elastic mechanics, the mechanical property of one object is mainly made of Young Modulus(E), bulk modulus(K), shear modulus(G), Poisson ratio(V) and Cauchy stress(C_{12}-C_{44}) etc. The amorphous region of PMIA cellulose was isotropic elastomer; for the substance made of isotropic material, only two elastic constants were required. Table 1 shows the mechanical properties in 2% moisture content at different temperature for PMIA system.

Table 1: PMIA mechanical property at different temperatures

Temperature / parameter	70℃	90℃	110℃	130℃	150℃
E	37.16	35.85	34.35	27.24	23.95
K	34.13	33.06	33.18	31.70	27.64
G	14.09	13.59	12.94	10.04	8.69
V	0.32	0.32	0.33	0.36	0.39
K/G	2.42	2.43	2.56	3.16	3.17
C12-C44	0.68	0.71	0.72	0.90	0.95

The increasing of tension modulus E value means the material rigidity and anti-deformation to be greater. The data analysis in Table 1 shows that the increasing temperature and decreased tension modulus can cause the anti-deformation capacity to be lessened; with greater shear modulus and material rigidity, the anti-deformation capacity would be better and elasticity would reduce. The table also indicates that the increasing temperature can decrease the shear modulus; the elastic modulus (E, K, and G) all relate to the material rigidness and anti-elastic property. Therefore, it is concluded that with temperature increasing, the values E, K and G reduce, i.e. rigidity is weakened, indicating that the temperature increasing can weaken the PMIA rigidity.

With higher Poisson ratio, the material plasticity shall be stronger, which was found by some previous literature to be related to the anti-shearing stability of the material. Cauchy (C_{12}-C_{14}) representation was material ductility: at negative value, the material exhibits brittle; at positive value, it exhibited ductile; and with greater value, the material plasticity shall be better. With greater ratio (K/G) of bulk modulus and shear modulus, the ductility shall be better: at value less than 1.75, the material exhibited brittle; at value more than 1.75, it exhibited ductile. Besides, the analysis of the temperature effect on PMIA Poisson ratio, K/G and Cauchy shows that with temperature increasing, the Poisson ratio, K/G and Cauchy stress all have an increased trend, i.e. temperature rise enhances PMIA plasticity and ductility.

3.1.2 Chain motion

To better understand the influencing mechanism of temperature on PMIA chain motion, the anhydrous complex model was selected as the research object. The statistics analysis for MSD for PMIA fibre chain was made as shown in Figure 2. Also, the radius of gyration (RG) was applied for further representing the influence of water and moisture on PMIA fibre chain. At last, by taking the average of the RG in the three chains, the results were obtained in Table 2.

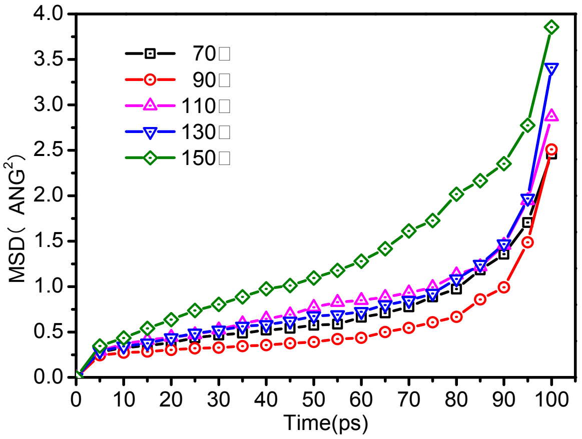

Figure 2: Mean square displacement of PMIA fibre at different temperatures

Table 2: The radius of gyration at different dimensions

Temperature (℃)	70	92	110	130	150
RG (1/ Å)	65.696	65.727	65.910	65.910	65.957

3.2 Moisture effect on PMIA performance

3.2.1 Mechanical property analysis of complex model

Tension modulus *E*, also be called as Young modulus, defined the ratio relation between uniaxial stress and uniaxial deformation, as the key indicator for material rigidness. Bulk modulus *K* stood for the relation between volumetric strain and mean strain of the object, in positive value. Shear modulus *G*, also called as rigidity modulus, indicated the ratio of shear stress and shear strain in the proportional region of elastic deformation, representing the anti-shearing capacity of the material. Table 3 lists the mechanical parameter in different moisture contents at 90℃.Table 3 lists the moisture effect on PMIA clearly: generally, with moisture increasing, the *E, K* and *G* of PMIA all have decreasing trend, showing that the PMIA rigidity and anti-shear capacity diminished gradually with the increased water molecule.

Table 3: PMIA mechanical parameters in different moisture contents

moisture / parameter	0%	1%	2%	3%	4%	5%
E	40.59	30.35	35.85	30.78	28.01	25.62
K	34.00	33.15	33.06	31.28	29.96	27.54
G	15.60	11.26	13.59	11.52	10.42	9.52
V	0.30	0.35	0.32	0.34	0.34	0.35
K/G	2.18	2.94	2.43	2.71	2.87	2.89
C_{12}-C_{44}	0.06	0.09	0.07	0.09	0.09	0.11

Poisson ratio *V* means the ratio of absolute value between transverse strain and axial strain, reflecting the elastic parameters of transversal deformation, and the plasticity & brittleness parameters of represented material as the dimensionless physical quantity. K/G reflects the toughness of material. The statistical analysis in Table 3 concludes, as the moisture content increases, the Poisson ratio, K/G and Cauchy all rises, indicating that the PMIA toughness and ductility has increasing trend with moisture content.

3.2.2 PMIA chain motion

Figure 3 depicts the MSD time variation curve for PMIA at 90℃ in different moisture contents. According to the changing trend, in lower moisture content, the MSD and moisture content has no obvious relations; but in 4% and 5% moisture content, the MSD of PMIA becomes greater with the reaction time increased, i.e. the chain motion of PMIA is relatively much intensified, which shows the thermal stability of PMIA is influenced in the moisture content 4% and 5%.

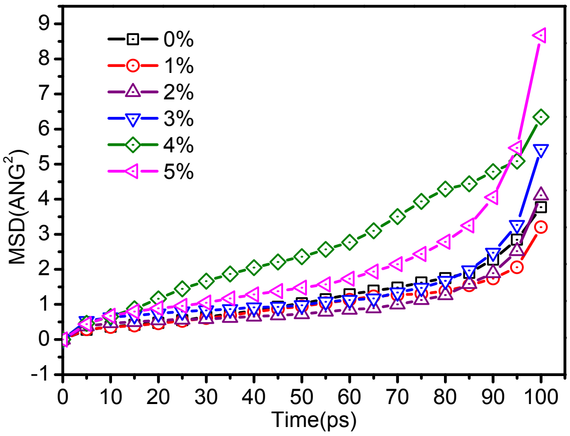

Figure 3: The mean square displacement of PMIA fibre in different moisture contents

4. Conclusions

Based on MD method, this paper makes simulation study of the PMIA complex model, and also analyses the temperature & moisture effect on PMIA mechanical property and thermal stability.

(1) The research results show, with temperature increasing, PMIA tension modulus, shear modulus and bulk modulus gradually diminishes, i.e. PMIA rigidity is weakened; the Poisson ratio, K/G and Cauchy also increase with temperature, indicating that the temperature rise enhances its ductility and plasticity; the mean square displacement of PMIA has the increasing trend with the temperature, and the radius of gyration increases with the temperature, showing the PMIA thermal stability is damaged with temperature rise.

(2) With moisture content increasing, PMIA tension modulus, shear modulus and bulk modulus gradually diminishes, i.e. PMIA rigidity is weakened; the analysis of PMIA mean square displacement shows that in lower moisture content, the PMIA molecular chain motion is unobvious; in higher moisture content 4% and 5%, the chain motion becomes more intensified, indicating the PMIA thermal stability to be lessened by the moisture.

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