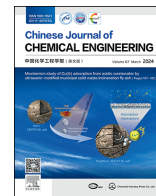




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Full Length Article

Alleviation of the plastic deformation of gel ink under strong stress through an esterification of xanthan gum reinforcing its double helix structure



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ABSTRACT

As a natural organic polymer, xanthan gum (XG) can alleviate the plastic deformation of gel ink under strong stress and realize the reasonable regulation of the rheological properties of gel ink. However, as the double-helix structure connected by hydrogen bonds cannot resist the mechanical environment of strong stress, XG shows poor shear resistance. In this study, a polymer gel with interpenetrating polymer network structure was prepared by esterifying XG, taking polystyrene maleic anhydride (SMA) as the modifier. In addition to retaining the excellent rheological properties of XG, the generated polymer gel also exhibited high shear resistance. The optimal addition amount of the esterification reaction modifier was determined as $m_{XG} : m_{SMA} = 5 : 3$ according to the gel ink standard. With this amount, the viscosity of the modified xanthan gum (SXG) gel increased to 1578.8 mPa·s and 100.7 mPa·s at shear rates of 4 s⁻¹ and 383 s⁻¹, respectively, and the shear resistance increased more than 2 times compared to the unmodified one. It is because of the ester bond formed by esterification that the reaction strengthens the interaction between molecular segments, enabling the new gel to resist to strong mechanical stress. The new polymer gel studied in this paper and the proposed mechanism of action provide new insights for the development of high-end gel ink and also provide theoretical support for the study of rheological properties of non-Newtonian fluids.

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1. Introduction

With the continuous improvement of the public use and awareness of gel pens, it has now become the mainstream product of writing instruments, and the production of gel pens will continue to rise in the future [1–3]. But due to the poor performance of the neutral ink, there are many problems with the writing of the filled gel pen, such as ink leakage, breaking, and ink accumulation, and their root cause is that the rheological properties of gel ink cannot match the strict writing requirements [4]. For decades, polymeric materials have shown a great potential in fluid

rheological regulation, and polymers can be divided into natural organic polymer compounds and synthetic organic compounds according to the source of the material. The researchers studied the interaction between various polymers with water molecules and pigment particles in aqueous systems and realized the rheological regulation of gel ink by constructing a dynamic network structure. Souza *et al.* [5] and Zhang *et al.* [6] introduced acrylic-based polymers, which use their unique polar group to form hydrogen bonds with water to show excellent water absorption performance and have a three-dimensional network structure to achieve the effect of water storage. However, because acrylic acid mainly relies on an alkaline environment to function, it has the problem of pH sensitivity. Du *et al.* [7] introduced polyurethane polymers; the imine group on the molecular chain and water molecules can form hydrogen bonds, and the weak polar polyester segments form physical cross-links and play the role of water storage, but the

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strong polarity and rigid urethane groups are easy to microscopically separate from the polyester chain segments due to their large molecular cohesion energy (see Table 1).

However, with the continuous improvement of the rheological properties and environmental protection requirements of gel ink, as well as the high cost of synthetic polymers, researchers have focused on natural organic polymers with excellent performance. Natural organic polymers are usually composed of thousands of atoms covalently bonded with each other to form organic compounds with particularly large relative molecular masses and repeating structural units. The polymer level is relatively large and usually has a tertiary structure. Its hydrogels have gel-like rheological properties [8], and it has strong plasticity, providing conditions for regulating the rheological properties of gel ink. Natural organic polymer compounds rely on the hydroxyl group on the molecular chain to hydrogen bond with water molecules adsorbing water molecules near the molecular chain, and the active groups on the molecular chain give polymer compounds a negative charge, the negatively charged side chain and the positively charged pigment particles attract each other to achieve the adsorption effect. Other than that, they rely on the intermolecular force and the winding and cross-linking of the molecular chain to form a “dendritic” network structure, hindering the free flow of water molecules and carbon-black particles. Based on the study of molecular aggregation structure, researchers proposed a phenomenological molecular aggregation model and elucidated the unique rheological behavior of natural organic polymer compound hydrogel system based on the equilibrium movement of molecular aggregation. In addition, the zero-shear viscosity calculated by the model is proportional to the concentration, which has a great influence on the process rheology and the resulting rheological response [9–12]. However, natural organic polymer compounds still have defects in mechanical properties [13], mainly manifested in large viscosity loss at high shear rates. Since the natural organic polymer compounds connect the rigid rod-like structure (primary structure) to form a double-helix structure (secondary structure) through intermolecular hydrogen bonding, whose bonding force is too weak to break after applying shear force [14], forming a plastic deformation of the double-helix structure failure under strong stress, and then showing that the viscosity of the system is greatly reduced. Sun *et al.* [15] and Wang *et al.* [16] modified natural organic polymer compounds to make them more resistant to shear forces and exhibit viscoelastic behavior. At present, the modification of natural organic polymer compounds is usually applied to oil extraction and binders [17] and is rarely reported in the field of gel ink. Therefore, exploring new multifunctional thickeners with potential prospects is the best strategy to achieve reasonable regulation of the rheological properties of gel ink.

The rheological properties of the gel ink prepared from this material are determined by the adsorption capacity of the polymer to water and the network structure formed by the cross-linking and entanglement of molecular chains, so finding a suitable natural organic polymer material is the key to achieve the control of the rheological properties of gel ink. As a natural polysaccharide, xanthan gum (XG) has a large number of hydroxyl groups in its molecular structure, which can adsorb a large number of water

molecules. In addition, the molecular weight of XG is large, and its unique double-helix network structure can better bind the flow of free water. These two aspects meet the requirements of the two units of the aqueous rheological system. At the same time, XG is widely used in food engineering, cosmetics, petrochemical, and pharmaceutical industries because of its good biocompatibility and non-toxicity and shows excellent rheological properties in these fields [18–21].

Inspired by this, we propose a strategy to construct an interpenetrating polymer network based on an esterified modified XG-reinforced double-helix structure [22], that is, to modify XG with the help of polystyrene maleic anhydride (SMA) to construct a new thickener with strong shear resistance [23]. In this work, the modified xanthan gum (SXG) was prepared by esterifying modified XG with different amounts of SMA, and the changes of XG before and after modification and the network structure before and after shearing were analyzed by infrared spectroscopy and metallographic microscopic characterization. Through the characterization of rheological properties combined with molecular dynamics (MD) simulation, the changes of rheological properties of the SXG system were analyzed, and the mechanism of action of the XG system was further determined. By studying the thickening mechanism of XG and the chemical modification of the molecular structure of XG, this paper provides new insights for the exploration of gel ink rheological systems, provides theoretical support for the study of how to regulate the rheological properties of non-Newtonian fluids, and also provides certain reference value and reference significance for many fields (such as food, industry, agriculture, oil extraction, pharmaceuticals, personal care, and home care).

2. Experimental

2.1. Materials

XG (food grade), carbon black (45 L), dispersant 96, and rust inhibitor (benzotriazole, AR) were purchased from the Guangdong Shunde Changhao Trading Co., Ltd, China. Preservatives (GXL, AR) were purchased from the Jining Xuli Chemical Co., Ltd, China. pH adjuster (triethanolamine, AR) and macrogol 300 (industrial grade) were purchased from the Dow Chemical Company, China. SMA (AR), dimethyl sulfoxide (DMSO, AR), tetrachlorofuran (AR), acetone (AR), and absolute ethanol (AR) were purchased from the Shanghai Yien Chemical Technology Co., Ltd, China. Deionized water was used for all polymerization and treatment processes.

2.2. Experimental methods

2.2.1. Preparation of modified XG

The XG was esterified with SMA as a modifier, as shown in Fig. 1. Approximately 5 g XG was added to 100 ml of dimethyl sulfoxide and stirred at 40 °C for 6 h to allow it to swell thoroughly. Next, a certain amount of copolymer of styrene and maleic anhydride was dissolved in 100 ml tetrachlorofuran and added to the system drop by drop with a constant-pressure drip funnel. The temperature was raised to 60 °C and held for 20 h. Then it was cooled to room temperature (25 °C) and suction was performed; filtered results were put into 100 ml acetone and stirred for 2 h, and the pellet was separated by suction, and it was washed four times with ethanol (per 100 ml). Finally, the product was dried under vacuum at 25 °C for 24 h according to the aforementioned methods.

We prepared a total of five samples, as shown in the table in the following.

Table 1
Dosage of different samples

Sample	XG amount added/g	SMA amount added/g
XG	5	0
SXG-1	5	1
SXG-2	5	2
SXG-3	5	3
SXG-4	5	4

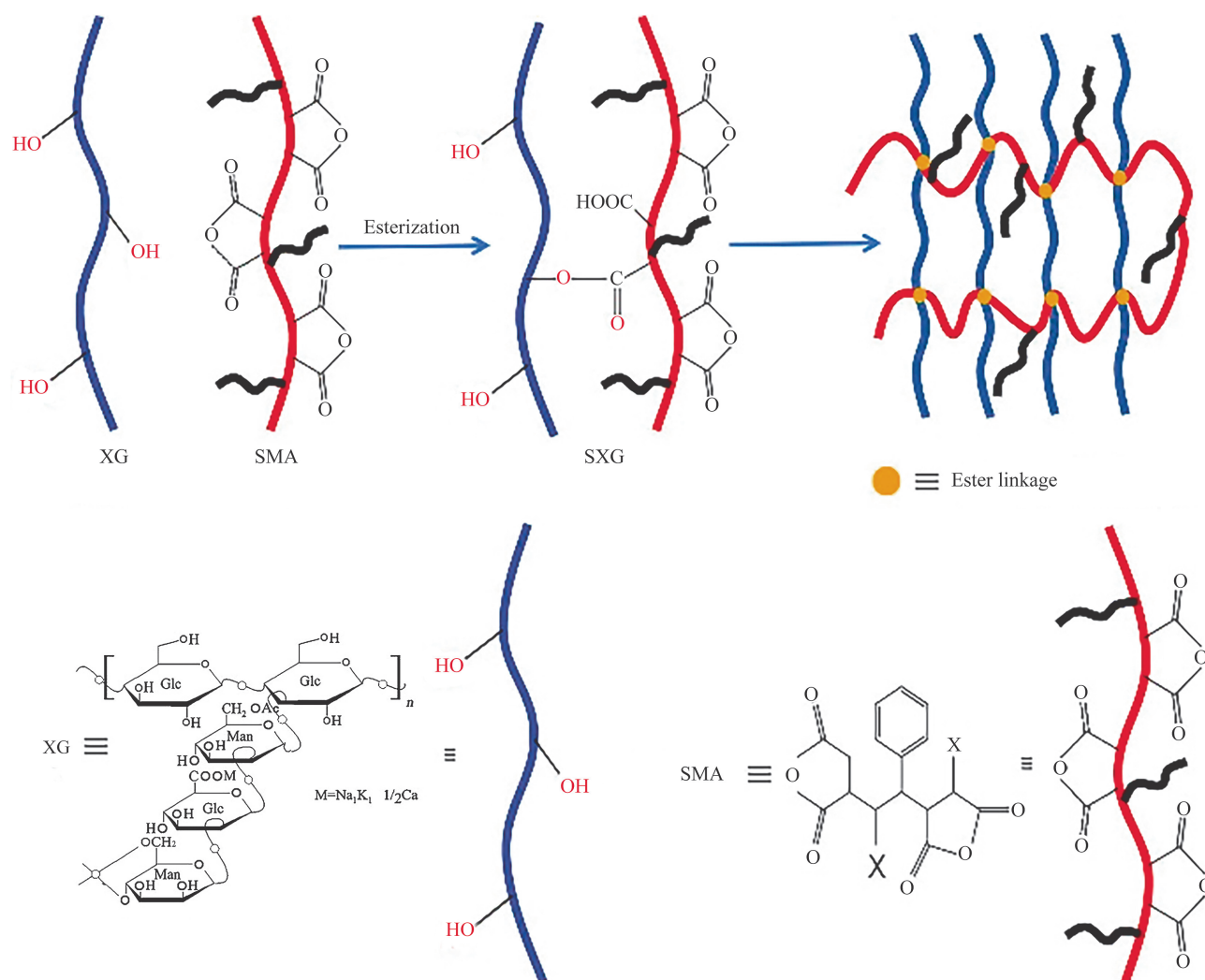


Fig. 1. Esterification of XG with SMA.

2.2.2. Preparation of gel samples

One hundred milliliter of deionized water was added to the beaker, then the same small amount of the samples prepared earlier was added to the beaker (added while stirring); finally, the mixture was stirred for 2 h and stood to obtain the gel samples.

2.3. Testing and characterization

2.3.1. Fourier-transform infrared spectroscopy

Fourier-transform infrared spectra were recorded with IS5 Fourier conversion infrared spectroscopy at 25 °C to characterize the molecular structure of the samples. For each sample, 16 scans were recorded between 4000 and 400 cm^{-1} , with a resolution of 4 cm^{-1} after tableted with potassium bromide.

2.3.2. Characterization of gel microstructure

The same appropriate amount of sample XG gel and SXG-1 gel were taken and coated evenly on the glass sheet, and the color paste liquid was dropped on the gel to exhibit the stained network structure. The M230-3M180 metallographic microscope of Shenzhen Osmicro Optical Instrument Co., Ltd., China, was used to observe their microstructures. An appropriate amount of the aforementioned gel samples was taken and sheared at high speed with a high-shear

mixed emulsifier, and then after shearing, the microstructures of the gel were observed by the same method.

2.3.3. Rheological property characterization

Rheological properties of the samples were characterized by using a R/S + Rheometer, a coaxial cylindrical rotational rheological instrumentation from Brook filed Engineering Experiment Co., USA.

The gel samples were measured to obtain the viscosity at different shear rates. The shear rate was set from 0 s^{-1} to 400 s^{-1} at a constant temperature of $(25 \pm 0.1)^\circ\text{C}$.

The fluid type is described by the Herschel–Bulkley model $\tau = \tau_0 + K\dot{\gamma}^n$, where τ is the shear stress; τ_0 is yield stress, which is the critical stress value that the fluid needs to reach or must exceed to start flowing, and the energy required to react to the fluid to start flowing; K is the consistency factor, which is used to indicate the fluidity of the fluid; n is the flow index, $n < 1$ indicates that the fluid is a pseudoplastic fluid, the smaller n , the easier it is for the fluid to be sheared and thinned, and the greater the pseudoplasticity; and $\dot{\gamma}$ is the shear rate.

The shear rate was set to 383 s^{-1} , and the shear time was 120 s at a constant temperature $(25 \pm 0.1)^\circ\text{C}$, and the gel samples were measured to obtain the viscosity at a constant shear rate.

2.3.4. Particle size performance characterization

The Topsize laser particle size analyzer of Zhuhai Omeike Instrument Co., Ltd. (China), was used to characterize the particle size performance of the samples. First, an appropriate amount of configured gel sample and a small amount of carbon black of the same quality were added in a beaker and stirred thoroughly to obtain a gel sample with carbon black. Next, the background of the laser particle size analyzer was adjusted to stability; the refractive index was set to 1.5, and absorbance was set to 1.0. Then 1 ml of the sample was diluted in a beaker with deionized water at the ratio of $V(\text{sample}):V(\text{water}) = 1:50$ and stirred evenly; the diluent was added to the particle size meter-injection system, and the sample's particle size and distribution were tested when the shading reached between 7 and 8. Finally, the D90 and D100 data were recorded to characterize the sample sizes that are the particle sizes corresponding to the cumulative particle size distribution of the sample to 90% and 100%.

2.3.5. Molecular dynamics characterization

The Material Studio (MS) software is used to build individual models of system molecules and for geometry optimization of the monomer models. Based on MD, a molecular composite model before and after modification was established to analyze the effect of XG modification on the microstructure of polymer materials. Then the corresponding shear force was applied to the system to obtain the viscosity at different shear rates. The simulation uses the COMPASS force field, which is suitable for the study of organic molecules, metals, metal oxides, and metal ions.

In this paper, the MS software was used to construct the monomer models of the system molecules: XG molecular monomer, SXG molecular monomer, and Na-ion monomer and then optimize the geometric structure of the monomer model [24], as shown in Fig. 2. MS was used to construct the model: the temperature was 25°C and the initial density was 1.5 g·cm⁻³; the XG model containing 2 XG molecules and 12 Na ions and the SXG

model containing 1 SXG molecule and 12 Na ions were constructed, and then the energy of the two molecular models constructed was optimized to obtain the lowest-energy molecular models, respectively.

3. Results and Discussion

3.1. Structural characteristics of esterified modified XG

Fig. 3 shows the infrared spectra of XG and SXG, and the absorption peak of SXG is more consistent with XG, indicating that the SXG retains the basic structure of the XG skeleton. As shown in the figure, the SXG and XG present a hydroxyl absorption peak at $\nu_{\text{O-H}}$ 3427 cm⁻¹, and it is significantly weakened [25], indicating that the intermolecular or intramolecular hydrogen-bonding force of XG decreased. The absorption peak of XG at $\delta_{\text{O-H}} = 1254$ cm⁻¹ is significantly weakened, and in comparison, with the ester carbonyl group of XG at $\nu_{\text{C=O}}$ 1732 cm⁻¹ [16], the SXG displaces at 1743 cm⁻¹. Both of these are mainly due to the esterification reaction that is the hydroxyl group on the XG molecule reacted with maleic anhydride to form an ester bond. Besides, a new carboxyl group absorption peak appears at $\nu_{\text{O-H}}$ 2345 cm⁻¹ because maleic anhydride opens to form a carboxyl group. Therefore, all of these indicate that the esterification modification is successful.

The microstructure changes before and after the modification of XG molecules are observed by metallographic microscopy, and the results are shown in Fig. 4. Through comparison, it is found that the microstructure of SXG changes significantly compared to that of protoxanthan gum. As shown in Fig. 4(a), it can be seen that a dense molecular network structure is formed when XG is in the gel state [26], which is also the reason why XG exhibits excellent rheological properties. Due to the presence of esterified modified XG, cross-linking occurs between molecular chains and forms a denser network structure as shown in Fig. 4(b). Fig. 4(c) and (d) are the phenomena observed by the microscope after high-speed shearing

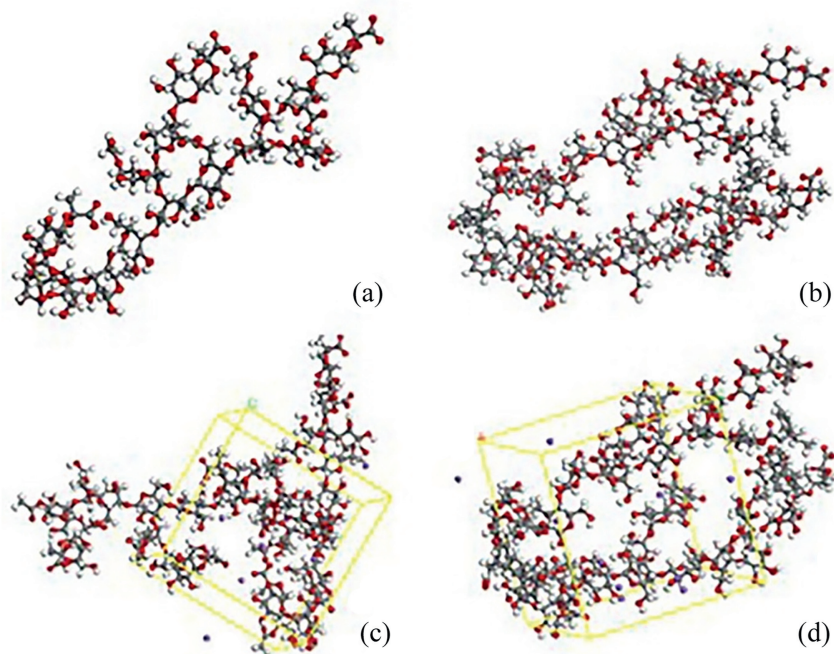


Fig. 2. Molecular model diagrams: (a) XG molecular monomer model, (b) SXG molecular monomer model, (c) XG molecular model, and (d) SXG molecular model.

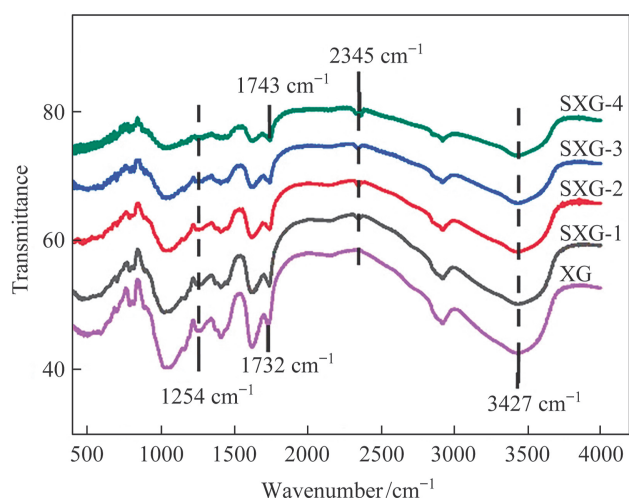


Fig. 3. Infrared spectra of XG before and after modification.

of XG before and after modification, and the high-speed shearing of XG will cause the molecular chain to break, forming many disordered, dispersed, spherical particles of different sizes and heights attached to carbon black [27]; however, the SXG still retains a part of the chain structure after high-speed shearing, which indicates that esterification modification strengthens the interaction between molecular chains.

3.2. Rheological and particle size performance of gels

Figs. 5 and 6 show the stable shear performance of XG and SXG gels at a constant temperature at 25 °C. It can be seen that the XG gel showed outstanding shear and viscosity reduction, that is, the most significant characteristic of a pseudoplastic fluid. This is because of the large molecular weight and long molecular segment of XG, which forms a huge spatial network structure through the intertwining of molecular chains, showing excellent rheological

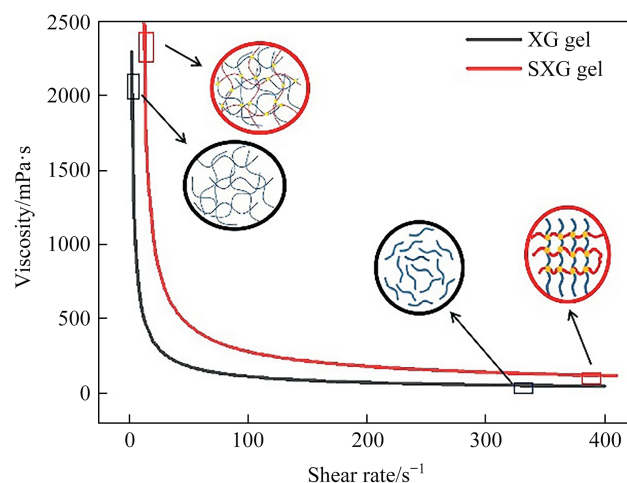


Fig. 5. Rheological conformational changes of gels.

properties [28]. The SXG retains the basic structure of the XG skeleton and still shows obvious thixotropy, and due to the cross-linking between the molecular chains of XG after modification, the molecular chain grows and the molecular weight increases, making the network structure denser and the shear viscosity higher.

The shear stress of the gels prepared before and after modification as a function of shear rate is shown in Fig. 7 (see Table 2). The Herschel–Bulkley model is used to fit the curve to obtain the equation $\tau = \tau_0 + K\dot{\gamma}^n$ [29]. The fitting results for the five samples are shown in the Table 3. As can be seen from the regression coefficient (R^2), the Herschel–Bulkley model fits very well. As can be seen in the table, n gradually decreases, and K gradually increases, indicating that the fluid exhibits more gel-like characteristics, and the microstructure of XG increases after esterification modification [30], and the strength of the three-dimensional structure increases (see Table 4).

The gels prepared by XG before and after modification were mechanically sheared at a shear rate of 383 s^{-1} , and the change of

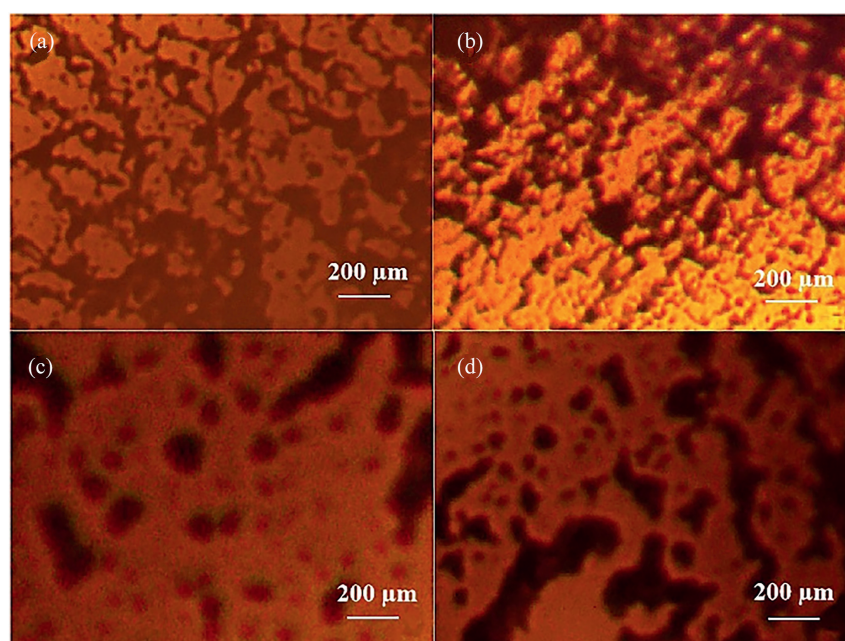


Fig. 4. Microstructure of gels before and after shearing at $50 \times$: (a) XG gel-before shearing, (b) SXG gel-before shearing, (c) XG gel-after shearing, and (d) SXG gel-after shearing.

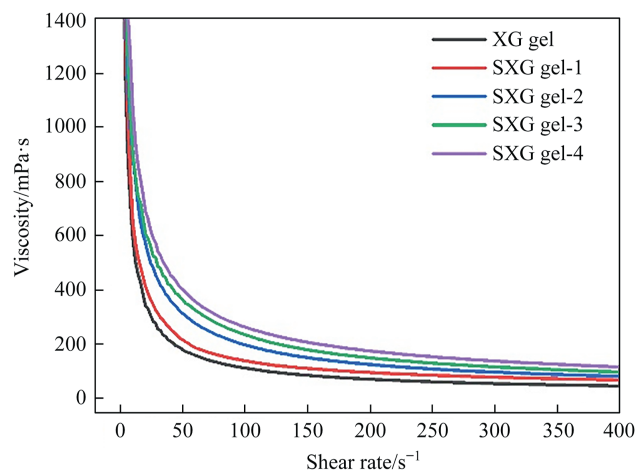


Fig. 6. Shear viscosity curve of gels.

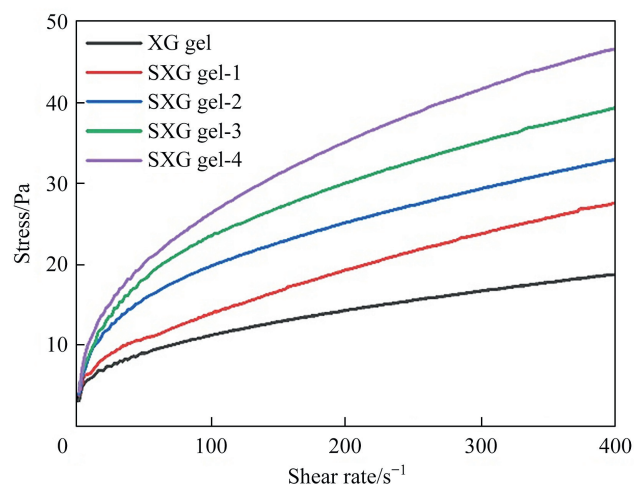


Fig. 7. Power-law model-fitting curve of gels.

Table 2

Functional groups and their corresponding infrared assignments

Wavenumber/cm ⁻¹	Functional group	Type of vibration
3427	Hydroxyl (O–H)	Telescopic
1254	Alcohol (O–H)	Bending
1732–1743	Lactones (C=O)	Telescopic
2345	Carboxylic (O–H)	Telescopic

Table 3

Fitting parameters for different samples

Sample	τ_0	K	n	R^2
XG gel	2.0001	1.3743	0.8425	0.9971
SXG gel-1	2.0825	1.9477	0.7783	0.9988
SXG gel-2	3.5217	3.5444	0.7129	0.9990
SXG gel-3	5.1469	4.3729	0.5487	0.9994
SXG gel-4	7.8356	4.8747	0.4156	0.9998

viscosity with shear time is shown in the Fig. 8. It can be seen from the figure that the viscosity of the gels decreased slightly with the extension of the shear time because a small number of molecular chains were broken at high shear rates. Moreover, the gels prepared by the SXG system show higher viscosity at the same shear rate, and with the increase of the degree of modification, the shear

Table 4

Comparison of samples' rheological data

Sample	Viscosity/mPa·s			Thixotropic value
	Shear rate 4 s ⁻¹	40 s ⁻¹	383 s ⁻¹	
XG gel	1193.9	211.9	48.1	5.63
SXG gel-1	1336.2	256.6	70.5	5.21
SXG gel-2	1484.7	360.2	84.4	4.12
SXG gel-3	1578.8	416.3	100.7	3.79
SXG gel-4	1686.8	454.3	119.7	3.72
Gel ink standard	1100–1600	250–450	90–110	≥3.5

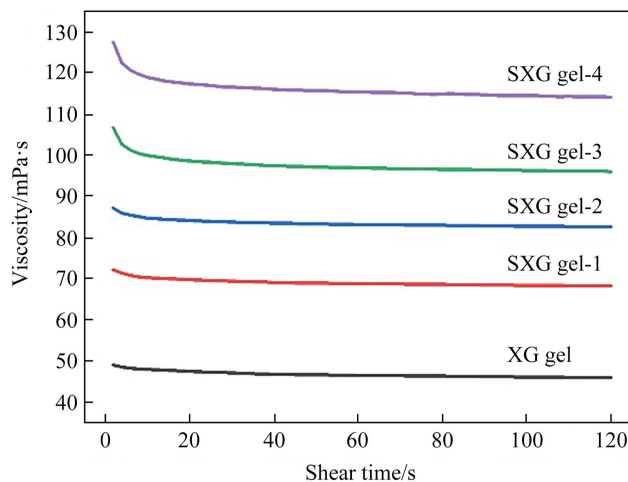


Fig. 8. High shear viscosity curve of gels.

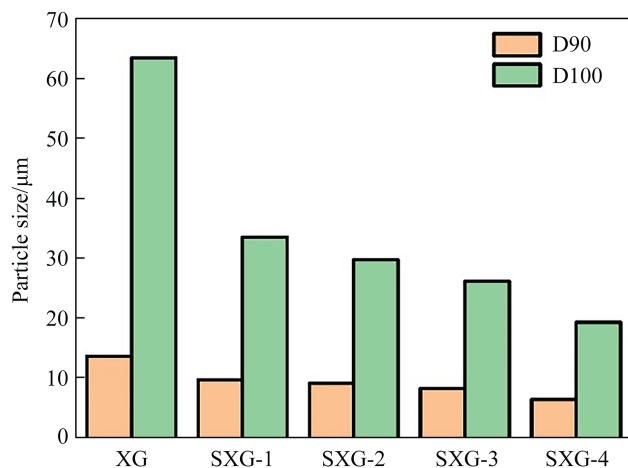


Fig. 9. Adsorption and dispersion particle size of gels to carbon black.

Table 5

Energy of different systems

System	Tol.energy/ kcal·mol ⁻¹	Pot.energy/ kcal·mol ⁻¹	Kin.energy/ kcal·mol ⁻¹
XG	120.479	–502.204	622.684
SXG	294.626	–424.874	719.500

Note: 1 kcal= 4.18 kJ.

viscosity also increases, indicating that due to the enhancement of ester bonds and hydrophobic associations, the micro-cross-linked structure in the polymer molecules increases so that the shear resistance of the system continues to improve [31].

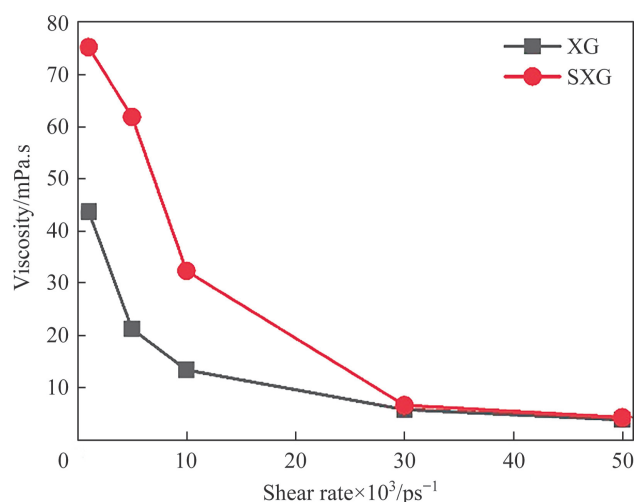


Fig. 10. Simulating shear viscosity.

In this experiment, the particle size and particle size distribution of XG and SXG gels dissolved with carbon black particles were studied. It can be seen from Fig. 9 that with the continuous increase of the amount of XG, the adsorption sites of carbon black particles on the molecular chain gradually increase, and the dispersion effect on carbon black particles also increases. Moreover, the dispersion effect of the SXG is significantly enhanced, which is due to the fact that the esterified XG molecular chain grafts with a large amount of styrene maleic anhydride, and the presence of the active-group benzene ring enhances the adsorption of the SXG on carbon black particles, thereby showing better dispersion ability [32].

The viscosity of the unmodified XG gel is $48.1 \text{ mPa}\cdot\text{s}$ at a shear rate of 383 s^{-1} , which is seriously lower than the standard value of the high-quality gel ink. This is the main problem of XG as a thickener. This problem can be significantly improved by esterification. When $m_{\text{XG}}:m_{\text{SMA}}$ is 5:1, the viscosity of the SXG gel at 383 s^{-1} increases sharply to $70.5 \text{ mPa}\cdot\text{s}$ but still does not meet the gel ink standard. When $m_{\text{XG}}:m_{\text{SMA}}$ is 5:3, the viscosity at 383 s^{-1} is $100.7 \text{ mPa}\cdot\text{s}$ and meets the gel ink standard. When $m_{\text{XG}}:m_{\text{SMA}}$ is

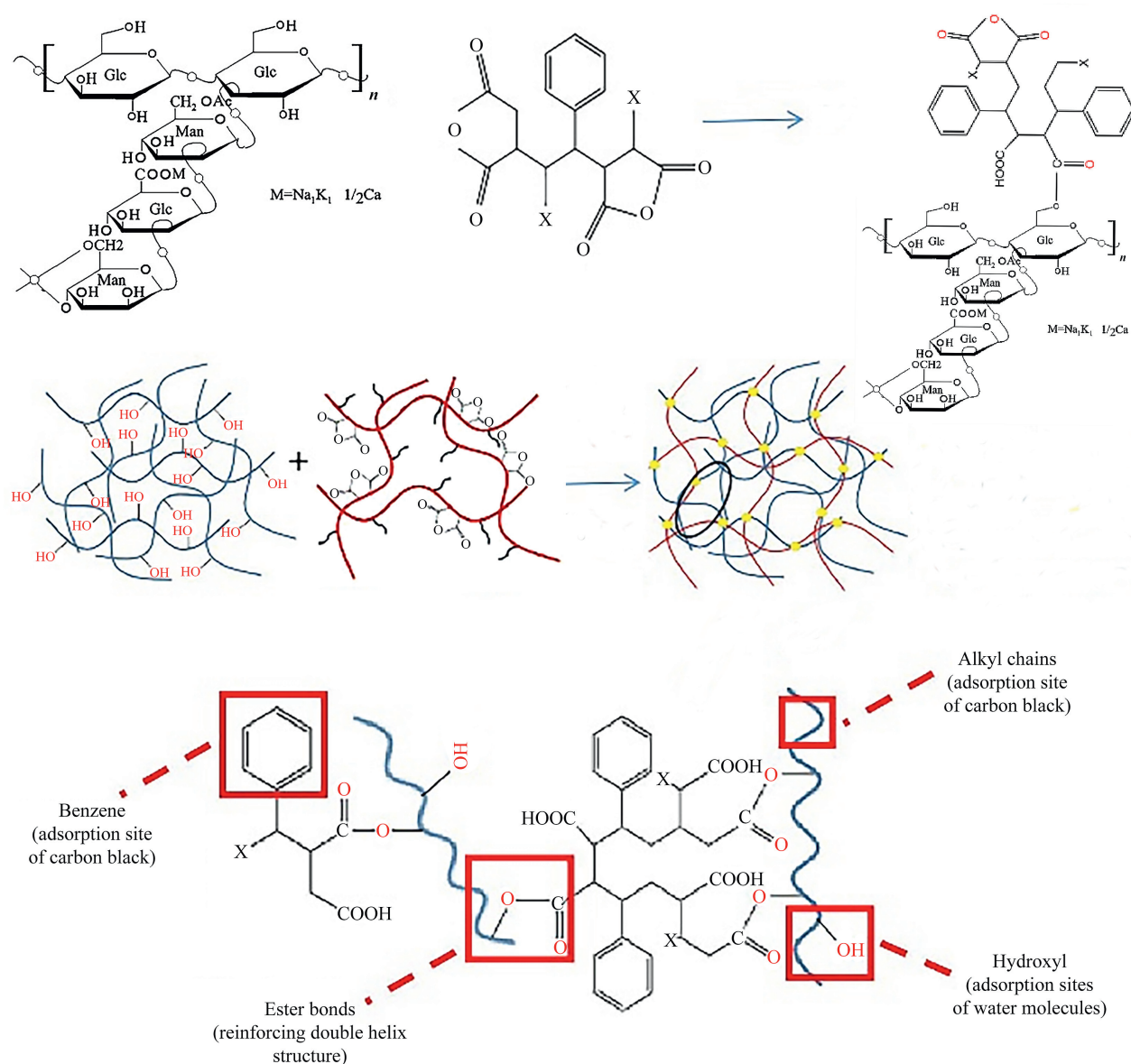


Fig. 11. Molecular mechanism diagram.

5:4, the viscosities at 4 s^{-1} and 383 s^{-1} are $1686.8\text{ mPa}\cdot\text{s}$ and $119.7\text{ mPa}\cdot\text{s}$, respectively, which exceed the gel ink standard. Therefore, the optimal addition amount of SMA should be $m_{\text{XG}}:m_{\text{SMA}} = 5:3$. With this addition amount, the viscosity of the SXG gel at a shear rate of 4 s^{-1} is $1578.8\text{ mPa}\cdot\text{s}$, and its thixotropic value is 3.79, all of which meets the gel ink standard.

3.3. Molecular dynamics simulation and mechanism analysis

In order to explore the molecular mechanism of esterification-modified xanthan collagen system, some attempts were made by MD simulation. The MD simulation of NVT at 200 ps was performed on the two lowest-energy molecular models at 25°C in steps of 1 fs to obtain molecular trajectory files with reasonable configuration and density. The entire simulation process in this paper uses the COMPASS force field [33], and the force field data of the system include total energy, potential energy, and kinetic energy. The microstructure of materials is an important internal reason affecting their properties, and it is also a prerequisite for the prediction and analysis of material properties. The energy of the system can be used to describe the interaction force of the molecular segments; the interaction force of the molecular segments has an important impact on the mechanical properties of the polymer: the stronger the interaction force, the closer the molecular segments of the material, the stronger the ability to resist deformation.

Energy analysis of the two polymer molecular systems at 298 K yields Table 5. Compared to the pure XG system, the total internal energy of the SXG-composite system is significantly improved, indicating that the interaction between molecular chains after modification is enhanced.

In order to eliminate the high-energy configuration of local molecular overlap and unreasonable structure, all systems first performed multiple energy minimization calculations, then used the NPT ensemble for density and pressure convergence, and finally, relaxed under the NVT ensemble to obtain the steady-state system structure. The shear rate was set to 0.001, 0.005, 0.01, 0.03, and 0.05 ps^{-1} , respectively, and the relevant physical properties of the system were calculated to obtain the shear viscosity performance of the two systems. It can be seen from Fig. 10 that both systems exhibit the characteristics of shear and viscosity, and the SXG system has higher shear viscosity, which is consistent with the previous rheological property characterization (see Fig. 11).

Natural organic polymer XG shows excellent rheological properties because of its unique tertiary structure. When the outside world applies high shear force, weak non-polar covalent bond is not enough to resist shear force; the change of XG tertiary structure from ordered state to disordered state makes the system viscosity drop rapidly. The esterification modification proposed in this paper makes a new ester bond form between the molecular chains of XG polymer, the energy of the system is enhanced, the force between the molecular segments is strengthened, the hindrance effect on the movement of water molecules is enhanced, and the viscosity is increased. On the other hand, the introduction of benzene rings in the modifier SMA increases the strong adsorption site of carbon black on the polymer molecule and enhances the adsorption capacity of carbon black.

4. Conclusions

In this paper, a new thickener was prepared by esterifying modified XG with SMA under heterogeneous conditions, and by comparing the infrared spectrum of XG before and after modification to observe the changes of its molecular structure, it was found that the SXG still retained the original skeleton structure, in addition to which, a new ester bond at 1743 cm^{-1} led to peak

displacement and a new carboxyl group absorption peak appeared at $\nu_{\text{O-H}} = 2345\text{ cm}^{-1}$, indicating that the esterification modification was successful. Secondly, by characterizing the microscopic morphology of XG gel and SXG gel before and after shearing, it was shown that the SXG formed a stronger network structure and that it retained a part of the chain segment structure after shearing.

Then, by characterizing the rheological properties of the gels, it was shown that the SXG gels exhibited high shear viscosity and excellent shear resistance, when $m_{\text{XG}}:m_{\text{SMA}}$ ratio is 5:1, the viscosity of the SXG gel at shear rates of 4 s^{-1} and 383 s^{-1} increased to $1336.2\text{ mPa}\cdot\text{s}$ and $70.5\text{ mPa}\cdot\text{s}$, respectively. The shear resistance of the gels was enhanced with the increase of SMA, when the $m_{\text{XG}}:m_{\text{SMA}}$ ratio was 5:4; the viscosity of the SXG gel at 383 s^{-1} was $119.7\text{ mPa}\cdot\text{s}$. The optimal addition amount of SMA was determined as $m_{\text{XG}}:m_{\text{SMA}} = 5:3$ according to the gel ink standard. With this addition amount, the viscosity of the SXG gel increased to $1578.8\text{ mPa}\cdot\text{s}$ and $100.7\text{ mPa}\cdot\text{s}$ at shear rates of 4 s^{-1} and 383 s^{-1} , respectively, and the thixotropic value was 3.79. Finally, the MD simulation method was used to construct the XG models before and after modification, and the kinetic analysis of their shear effect was carried out, and it was concluded that the molecular segment of the SXG had enhanced intramolecular energy, increased intermolecular force, and it exhibited higher viscosity than XG after shear force was applied, which was consistent with the rheological characterization results.

Declaration of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data Availability

Data will be made available on request.

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