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### Application of Infrared Spectroscopy in Biomedical Polymer Materials

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#### 1. Introduction

Infrared Spectrum (IR) is mainly used to study molecular structure and composition in substances and thus is also called molecular spectrum. When the sample is exposed to infrared light with continuously changing frequency, the molecule absorbs irradiation of certain frequencies and is subject to vibration or rotation, thus to cause the change of dipole moment. The molecule's transition from normal state to excited state weakens the intensity of the corresponding transmitted light in the absorption region, then the infrared software is used to obtain the IR spectrum. Started in 1970, Fourier Transform Infrared Spectroscopy (FTIR) was of high resolution and high scanning speed. It was not only limited to middle infrared (MIR), Spectrum ranges ultraviolet to far infrared section with the assistance of the beam splitter. The main direction of modern analysis, study and development is to combine technology of FTIR with that of the other instrument. For example, FTIR-TGA (Thermogravimetry Analysis) can be used to obtain the real composition of vapor generated in the various weight loss stages and the decomposition process.

Ultraviolet and visible absorption spectrum are usually used to study unsaturated organic matter, especially the organic compounds with conjugated system. However, infrared spectroscopy mainly studies chemical compounds with change of dipole moment during vibration. Thus, almost all organic compounds, except single atoms and homonuclear molecule, absorb in the infrared spectrum region. Except for optical isomers, some high polymer of high molecular weight and compounds with slight difference in molecular weight, two compounds of different structure are unlikely to have the same infrared spectrum. Wave number position, number of wave peaks of infrared absorption band and the intensity of absorption band indicate the characteristics of the molecular structure, and thus can be used to identify the structural composure of the unknown objects or its chemical groups. The absorption intensity of the absorption band is related to the contents of the molecular composition or the chemical groups and can be used for quantitative analysis and purity identification. Infrared spectrum analysis has distinctive characteristic and can be used to test gas, liquid and solid samples. Lie other analysis methods, it can be used for qualitative and quantitative analysis and is one of the effective methods for chemical compound identification and molecular structure elucidation.

#### 2. Summary of biomedical polymer materials

Biomedical polymer material is an important component of biological material and is a remarkable functional polymer. It involves in physics, chemistry, biochemistry, medicine, pathology subjects. The synthetic polymer materials and the organisms (natural polymer) have a very similar chemical structure, which determines their similarity in performance and enables high molecular polymer to meet the many complicate and rigorous functional requirements for medical products. Most metal and inorganic materials are incapable in this respect. Presently, high molecular polymers are widely used in medical products.

## 2.1 Presently there are two types of high molecular polymers: Non-biodegradable and biodegradable polymer materials

Non-biodegradable biomedical polymer material is widely used in manufacturing of adhesives, coating, and artificial lens as well as for repair of the many soft and hard tissues and organs of human body such as ligament, tendon, skin, blood vessel, artificial organs, bone and teeth. Most non-biodegradable biomedical polymer materials have no biological activity and are difficult to bond firmly with tissues and thus may result in toxicity and allergic reaction. Biodegradable biomedical polymer material is mainly used in temporary execution and replacement of tissue and organ functions in clinic or be used as the medicine controlled-release system and delivery carrier, absorbable surgical suture and wound dressings. It is readily biodegradable and the degradation products can be excreted through metabolism. Thus, it has no negative effect to tissue growth. Presently, it has become the key focus in development of biomedical polymer materials.

| Non-biodegradable Polymer Materials      | Biodegradable Polymer Material                        |  |  |
|--|---|--|--|
| Silicone Rubber<br>Polyethylene          | Polyvinyl alcohol<br>Modified natural polysaccharides |  |  |
| Polyacrylate                             | Protein   |  |  |
| Polytetrafluoroethene -PTFE, etc.        | (Back spinning) synthetic polyester                   |  |  |
| Dacron                                   | Polypeptide-polyolefine, silk ossein                  |  |  |
| Carbon-graphite fiber, etc.              | PLA   |  |  |
| Table 1. Category of Biomedical Polymers |   |  |  |

However, biomedical polymer is an interdisciplinary subject and has varying types of classification based on different purposes and practices. For example, it can be categorized based on the source and application purpose of the medical polymer or based on the influence of living tissues to the materials. Presently there is no uniform standard for the classification.

#### 2.2 Biomedical polymer material

Polymer material is generally composed of high polymers and low molecular weight substances. High polymers are divided into homopolymer, copolymer, blends and oligomer; Low molecular weight materials include: 1) additives: regulator, chain transfer agent,

terminator and emulsifier; 2) additives: plasticizers, stabilizer, filler and colorant etc.; 3) unreacted monomer, residual catalyst, etc.

Compared with ordinary organic substance, polymer-a long chain connected by multiple monomer units through covalent bonds—features diversified and designable structure, with very high mechanical strength and non-fixed molecular weight. Polymer is partially crystallized or non-crystallized and provides the properties of elastomer and fluid.

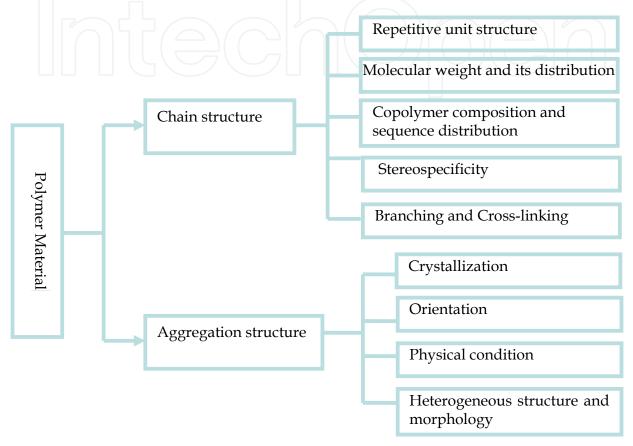


Table 2. Polymer materials

#### 2.3 Basic requirements of biomedical polymer and common materials

Biomedical polymer is directly applied to human body and is closely related to human health. Therefore, the materials used for clinic should be strictly controlled, otherwise, it may cause adverse effect instead of life saving. Below are requirements on properties and performances of the biomedical polymer:

- 1. Resistance to biological aging: polymer for long-term implantation should have good biological stability.
- 2. Physical and mechanical stability: different strength, elasticity, size, stability, fatigue resistance and wear resistance for different application.
- 3. Easy for processing and molding
- 4. Proper materials with reasonable cost
- 5. Convenient for sterilization.

Requirements on body effect of biomedical polymer

- 1. Non-toxic, i.e. chemically inert
- 2. No pyrogenic reaction
- 3. Non carcinogenic
- 4. Non-teratogenic
- 5. Does not cause allergic reaction or interfere with the body's immune mechanism
- 6. Does not damage adjacent tissue or cause calcified deposition on material surface.
- 7. Excellent blood compatibility without causing coagulation when contacting with blood.

Requirements for biomedical polymer production and processing: besides the strict control on biomedical polymer itself, matters harmful to human body shall also be prevented during material production; the purity of the raw materials used in biomedical polymer synthesis shall be strictly controlled, no harmful matter is allowed and the content of heavy mental shall be within the limit; additive processing shall meet medical standard; the production environment should meet proper standard for cleanliness.

The commonly used biomedical polymer materials include Polytetrafluoroethene, polyurethane, polyvinyl chloride, silicone rubber, polypropylene, polysiloxane gel, poly methyl acrylate, chitin derivatives and Polymethylmethacrylate.

#### 2.4 Biomedical polymer material study content

Structure-property relationship: different materials have different properties; the same kinds of materials have different properties; the property of the material not only relevant to its composition but more importantly is relevant to its structure. Moreover, its basic performance and processing performance are sometimes inconsistent with its operational performances.

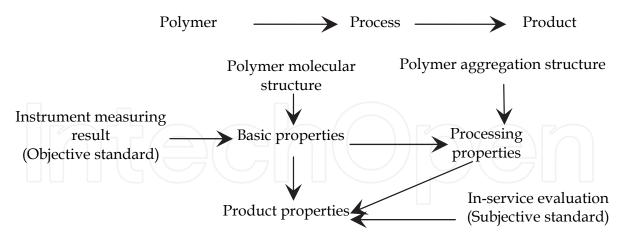


Table 3. Structure-property relationship of Polymer Material

#### 2.4.1 Polymer chain structure study

1. Polymer-based band

Most bands in the spectra are characterized by small molecule band with structure similar to repetitive units, i.e. elemental bands; also there are some unique absorbing bands different

from the small molecular organism that belongs to polymer-based bands. Conformation bands; Stereoregularity bands; Conformational regularity band; Crystal band

Such bands are of great significance to the study of polymer.

- 2. Determination of chemical composition
- 3. Determination of degree of branching
- 4. Determination of copolymer composition
- 5. Determination of the sequence distribution of the copolymer
- 6. Influence from additives

Adding modifier into certain materials may obtain new material with different performances. But the difference of the infrared spectra maybe small.

#### 2.4.2 Change of polymer materials

Monomer – polymer – Products – Application

#### 2.4.3 Analyses on polymer material

Development of new materials, assimilation of introduced technology and gradual internationalization; discrimination of true and false materials

#### 3. Characteristics of polymer IR spectrum

Infrared spectroscopy is the most effective method to identify the various polymers and additives in polymer material analysis. The main advantages of the infrared spectroscopy include: 1) it does not cause damage to the sample under analysis; 2) it may analyze organic and inorganic compounds of various physical states (gas, liquid and solid) and various exterior forms (elastic, fibrous, thin film, coating and power form); 3) well-developed molecular vibration spectroscopy (the basis of IR spectrum) makes it easy to understand the explanation of the IR spectrum of the compound; 4) a large number of standard infrared spectrogram for various kinds of chemical compounds have already been published in the world and can be referred to in spectra analysis. With application of computer and establishment and improvement of spectral database, the spectral identification will be easier and conclusion will be more reliable. Chemical compounds of different chemical structures have infrared absorption spectroscopy of different characteristics, There is no completely identical spectroscopy except for some isomers. Moreover, each absorption band (band) in the infrared spectrogram represents a certain vibration type of a certain atomic group or radical in the chemical compound. Their vibration frequency (corresponding to the wave numbers of the absorption band on the spectrum) is directly related to the mass and chemical bond strength of the atom in the atomic group or radical. They are consequently subject to changes of proximity structure and different influences of chemical environment. As each molecule of the polymer contains a great number of atoms, it may be considered that the polymer spectrum would be extremely complicate with considerable number of normal vibration. But this is not the case, IR spectra of some polymers are more simple than that of the monomers. This is because polymer chain is made of many repetitive units and each repetitive unit has basically same bond force constant with roughly similar vibration frequency. Moreover, due to limitation of strict selection law, only part of the vibration has

infrared activity. The explanation of infrared spectrum of polymer must take into account the molecular chain structure and the aggregate structure of the concerned polymer. Different structural characteristics correspond to different absorption bands: ① absorption bands: reflects the chemical composition of polymer structural unit, connection type of monomers, branching or cross-linking and sequence distribution. ② Conformation bands: such bands are related to the certain conformation of some radical in the molecular chain and have different representations in different morphologies. ③ Stereoregularity bands: these bands are related to the structure of the molecular chain and are therefore identical in the various morphologies of the same high polymer. ④ Conformational regularity bands: these kinds of bands are generated as result of the mutual action of the adjacent radicals in the molecular chain. ⑤ Crystal bands: the bands are formed as a result of the interaction between the adjacent molecular chains in the crystal.

#### 4. Preparation of samples

In order to obtain high quality infrared spectra, a proper method should be selected for sample preparation according to the characteristics of the sample. Close attention should be paid to the following in sample preparation: 1) Purified and separated sample. IR spectrum of mixed sample will be shown in bands of various components and may mislead judgment for the sample. 2) Free of moisture. The infrared spectroscopy is very sensitive to moisture. If there is any trace of moisture in the sample, bands with intensive OH radical characteristic will be appeared near 3400cm<sup>-1</sup>, affecting the identification of N-H, C-H bonds. 3) Proper concentration and thickness of the sample. In good infrared spectra, most of the absorption bands have transmittance of between 20 to 80%. In especially low concentration or thin thickness, weak absorption bands and band of medium strength will disappear, resulting in inaccurate absorption spectrum. On the contrary, the excessive strong absorption will result in flat peak with no maximum value of the peak or indistinct double peaks.

#### 4.1 Solid sample preparation technology

Common solid samples include polymer and some organic compounds. The following methods are usually adopted for sample preparation:

- 1. Pressed halide disk method (KBr Pressed Disk Method), mix a quantitative amount of samples (accurately measured for quantitative analysis) And some ground and screeened KBr powder in the agate mortar in proper proportion and pulverize them completely until there is no obvious particles in the blends. Please be noted: KBr requires the use of analytical reagent or higher. Qualified KBr should be no absorption in mid-infrared region. Moisture absorption will result in moisture absorption peak. In addition, KBr powder tends to absorb the vapor in the air and should be dried before use. Screen the KBr powder with 200-mesh sieve, then dried under 120°C and put the powder in the dryer for use. The temperature should not be too high(greater than120°C), otherwise it will decompose (see spectra 1).
- 2. Paste Method

#### Sample Preparation

Put the fully grounded powder sample in the agate mortar, add 1-2 drops of medium by dropper and blend evenly. Use stainless steel spatula to scoop out the evenly grounded

sample, paste it on a window slice, compress with another window slice to a proper thickness and then measure it.

Notes:

All the media used in the method are organic matter and can absorb in certain range. The absorption positions of the media are as shown below:

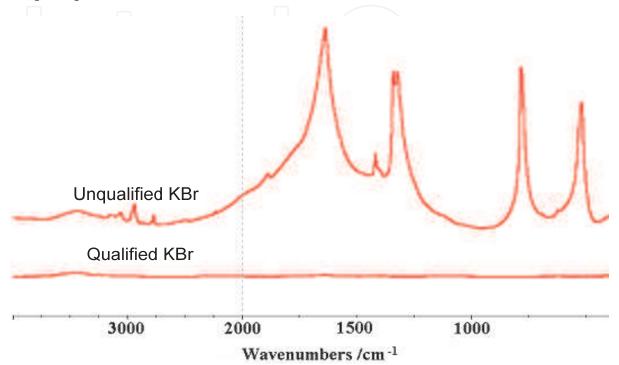


Fig. 1. Absorption requirement of qualified KBr

| Name of media                        | Absorption peak location and assignment  |  |
|--------------------------------------|--|--|
| Paraffin oil (long-chain alkane)     | 3000-2850cm <sup>-1</sup> (V <sub>C-H2</sub> , V <sub>C-H3</sub> )                     |  |
|                                      | 1468 cm <sup>-1</sup> , 1397 cm <sup>-1</sup> (δ <sub>C-H2</sub> , δ <sub>C-H3</sub> ) |  |
| Fluorocarbon oil (perfluoroparaffin) | With C-F absorption of different intensity in  |  |
|                                      | 1400-1500 cm <sup>-1</sup>   |  |
| Hexachlorobutadiene (chloroalkene)   | With C=C and C-Cl absorption in 1500-16010   |  |
|                                      | cm <sup>-1</sup> , 1150-1200 cm <sup>-1</sup> , 600-1000 cm <sup>-1</sup>              |  |

Table 4. The absorption positions of the media

The IR spectra of above three media have complementary. Complete infrared spectrogram of the sample can be obtained by at least two media. In this consideration, the influence of the media spectrogram should be deducted from spectrum analysis of the sample to baseline.

3. Solution film casting method

Sample preparation method

Dissolve the sample in an appropriate volatile solvent to prepare a solution with concentration of around 2-5%, apply the solution evenly on the watch glass and glass sheet,

or drop it directly on the infrared wafers (KBr, NaCl, BaF etc), then solvent volatilize to obtain sample film.

Application Scope: mainly used in sample analysis with both film-forming and solvent dissolving.

Notes:

The selection of solvent and the concentration of the sample prepared play an important role in obtain even and pure film.

Principle for Solvent Selection:

All solvents have infrared spectrum absorption band. Commonly used solvent oil include  $CCl_4$ , CH  $Cl_3$ , CS<sub>2</sub> and n-hexane.

Select solvent with low boiling point instead of using solvent with high boiling point and strong polarity, otherwise, the film thickness will be uneven as result of the fast solvent volatilization.

The solubility of the sample in the solvent should be sufficient high. The solution concentration can be regulated.

4. Hot-press film making method

Hot-press device: composed of hydraulic membrane machine, heating die and temperature control device.

Hot-press temperature setup for various common polymers

Sample preparation method

Place a piece of aluminum foil in the core of the die, put the sample on the aluminum foil and then place another piece of aluminum foil on the sample; put on the upper module and then place the die on the tablet press. Control the pressure within 1000-3000Kpa/cm<sup>2</sup>. The heating temperature and time for pressing shall be controlled to the extent that there is no thermal decomposition or other chemical changes. After pressing for about 1min, take down the die from the hydraulic press (wear insulating glove to avoid burn), cool to room temperature and then unpack the die to take out the sample tablet. Reduce sample volume if the film is too thick. Reduce temperature if the film turns yellow or has bubbles. Uneven film is caused by low heating temperature, too short heating time or small pressure. Reselect film making condition to remake the film in case of any of the above circumstances.

Application Scope: applicable for non-oxidizing and non-degradable thermoplastic or inorganic polymer materials near the softening point or melting point.

Notes:

Select appropriate hot pressing temperature and pressing time according to the nature of the analyzde sample in order to obtain hot press film in line with infrared transmittance while not destroying structure performance of the sample. Take protective measure against burn when operating in high temperature.

General solid sampling technique can be used in the infrared analysis. However, improvement has been made in actual operation based on the features of the polymer. Mr.

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Yang Rui from Tsinghua University has made a detailed research and analysis (in 2011) as below:

**Thermoplastic resin:** dissolve flow casting film, hot-pressing film or dissolve coated tablet.

**Thermosetting resin:** such as curing epoxy resin and phenolic resin. Use clean steel file to file sample powder and then use KBr pellet.

**Mild cross-link polymer:** sample that only swells instead of dissolving in solvent. Grind with KBr in swelling (with solvent) condition, then dry the solvent and pulverize the tablet.

**Fiber sample**: Filament with diameter of less than 10 microns can be neatly arranged (or be cut into piece) to determine the transmission spectra with KBr pellet. Filament with larger diameter or non-filament fiber should be entangled on the aluminum tablet or be squashed for determination with ART.

| Polymer   | Temperature<br>/°C | Polymer                       | Temperature<br>/°C |
|---|--------------------|-------------------------------|--------------------|
| High-density polyethylene<br>Low density linear<br>polyethylene | 170                | Nylon 11                      | 220                |
| Low density polyethylene  | 150                | Nylon 66                      | 280                |
| Polypropylene   | 200                | Metaformaldehyde              | 190                |
| Polystyrene   | 130                | Makrolon                      | 260                |
| PMMA  | 260                | Polybutylene<br>terephthalate | 290                |
| PVC   | 190                | Polybutylene<br>terephthalate | 250                |
| Nylon 6   | 250                | Teflon                        | 360                |

Table 5. Reference Temperature for Hot-pressing Film of Common Polymers

Figure 2 shows PMMA infrared spectrum from different sample preparation methods. The PMMA infrared spectrum from powder pulverized tablet and hot-pressing film are nearly same on wavenunbers, and slightly different on wave intensity. But there is another additional infrared eigen wave (at 760 cm<sup>-1</sup>) for PMMA infrared spectrum from solution film casting method (chloroform resolving).

#### 4.2 Liquid sample preparation technology

#### 4.2.1 Material of window slice used for organic liquid testing

KBr and NaCl are the most commonly used window slice materials used for determination of IR spectrum of the organic solution. But KBr is widely used than NaCl. KBr is the most suitable window slice material for testing organic liquid in middle infrared.

Rinse the KBr wafer immediately after testing. As KBr is non-dissolvable with in soluble, remove the organic solvent from the surface of the wafer by anhydrous ethanol instead of clean water, then dry with crystal-tipped tissue.

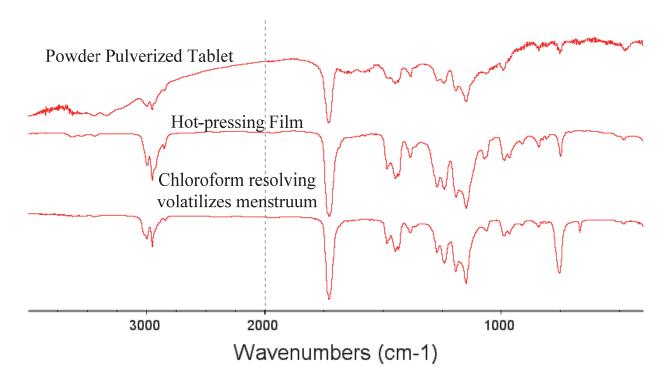


Fig. 2. PMMA Infrared Spectrum from Different Sample Preparation Methods

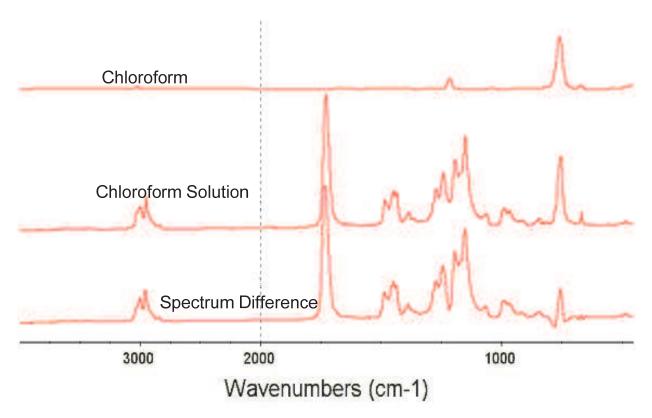


Fig. 3. PMMA Chloroform Solution and Difference Spectrum of Chloroform

#### 4.2.2 Window slice for testing aqueous solutions

The most commonly used Window slice materials for IR spectroscopy of aqueous solution samples is BaF2 wafer, followed by CaF2 wafer. Though BaF<sub>2</sub> wafer is non-dissolvable in water, it can be dissolved in acid and ammonium chloride and can react with phosphate and sulfate to generate barium phosphate or barium sulfate respectively, thus erode the surface of the wafer. When testing metal salt solution, the metal ion will exchange with barium ion and thus erode wafer surface.

#### 4.2.3 Preparation technology for liquid samples with different boiling points

1. Liquid with low boiling points

As the sample has low boiling point, a sealed tank should be used to prevent evaporation of sample. The thickness of the liquid membrane is decided by the nature of the sample. The stronger the polarity, the thinner the tanker is.

2. Liquid with high boiling point and low viscosity

Liquid sample with high boiling point, good flow property and low viscosity may be dropped between the two window slices of the removable liquid tank, then compress the automatically formed even liquid film for measurement.

3. Sample with high boiling point and high viscosity

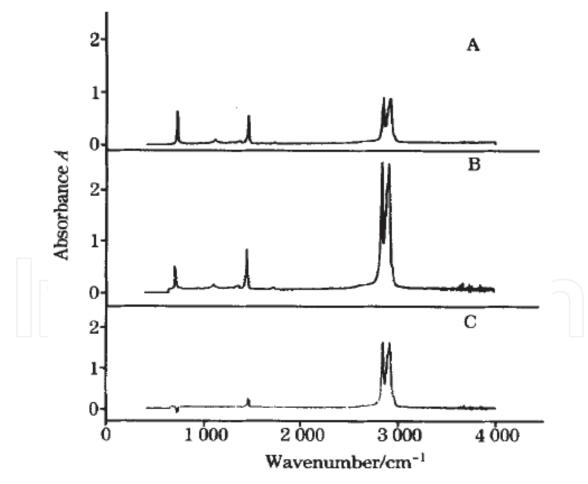
For qualitative analysis of plasticizer and pyrolysates used in the samples with high boilling point and high viscosity, such as grease, polymers, apply a small amount of sample on KBr window slice by stainless spatula, and scrape evenly, then put it on the sample rack for measurement.

#### 5. Analysis of infrared spectroscopy in biomedical polymer material

The key difference between medical polymer material and other polymer materials is that the former has both medical functionality and biocompatibility and resorts to chemical or physical means to achieve polymeric modification of polymer materials. Fourier Transform Infrared Spectroscopy (FT-IR) is an effective method to analyze polymer materials and its modification.

5.1 The transformation degree of dental composite resin after polymerization may directly affect the biological, chemical and mechanical strength. The most urgent problem in the application and development of the composite resin material is to remove various unfavorable factors that may affect solidification of the composite resin to maximize its transformation degree. FTIR spectroscopic technology may comprehensively study the polymerization of chemical curing and visible-light curing composite resin and the influences of various factors to the degree of polymerization as well as the relationship between transformation degree of the composite resin and the various indirect indicators. The existing study on FTIR indicates: Of different brands of dental composite resin available in market, the transformation degree of visible-light curing resin is superior to that of the chemical-curing resin; the double bond transformation degree and the mechanical properties of the resin have positive correlation with the contents of the catalyst and the reductive and have negative correlation with the contents of the inhibitors.

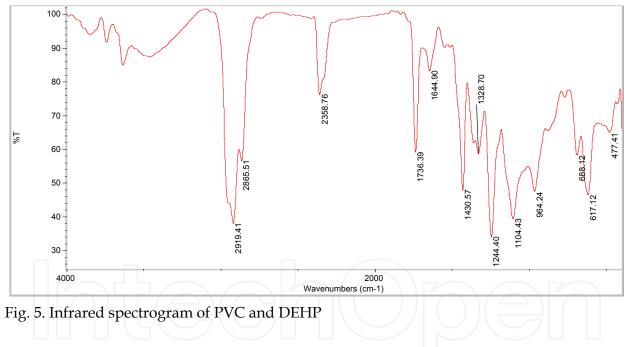
5.2 As the polymer surface properties affect the cohesiveness, wettability and biocompatibility of the polymer and its actual application, the study focusing on improving polymer properties through polymer surface modification. The quantitative analysis of the polymer surface composition is the important basis for the property study. Attenuated total reflectance infrared spectroscopy (ART-FTIR) technology is one of the most effective methods to test the information of the material construction of the polymer surface without interference of the test samples. Just as transmission infrared spectrum, ATR-FTIR provides information <sup>[1-5]</sup> about chemical structure, three-dimensional structure, molecular orientation and hydrogen bond of the material. The existing study<sup>[6]</sup> uses attenuated total reflectance Fourier transform infrared spectroscopy (FTIR-ATR) to test the surface composition of polyethylene glycol/ polyethylene blends (PEG/PE) film. With the corresponding characteristic peak intensity ratio as the basis for the quantitative determination, ATR correction procedures, and NMR-FTIR correction equation<sup>[6~7]</sup>: Y=0.346 48-1.336 55X+1.268 37X<sup>2</sup>, are used for quantitative analysis of the relative composition of the polyethylene glycol chain and the polyethylene chain on the blend surface to obtain a better result of the reproducibility and comparability. The quantitative analysis of the relative composition of polyethylene glycol chain and the polyethylene chain on the surface layer of the blend film is achieved through working curve method. See figure as below:



A. ATR spectrumwithout calibration; B. Corrected ATR spectrum; C. The difference spectrum between spectra A and B Fig. 4. ATR spectra of blend of PEG (2000) and LLDPE

5.3 Another key focus of study is to use combined infrared spectroscopy and computer technology to make quantitative analysis of the chemical structure of the auxiliary materials added to the medical polymer, such as additive, adhesives and plasticizer. Spectrum subtraction technology can be used to identify the additives in the high polymer products. Medical infusion devices are made of conventional polymer material polyvinyl chloride (PVC) and 2-ethylhexyl phthalate (DEHP) is added to plasticize rigid polyvinyl chloride (PVC), with additive dosage of 40-60%. Study has verified that DEHP can enter human body through venous transfusion, respiratory tract and skin and bring damage to human health. This has become focus of academic research and disputes and has attracted attention from media. Though DEHP's toxicity and carcinogenicity has been fully confirmed in experimental animals, its adverse effect in human body is still controversial. Using infrared spectroscopy subtract technology to analyze PVC infrared spectrogram of PVC and the infrared spectrogram of plasticized PVC may determine the kernel of material construction of the plasticizer. FTIR spectrum subtraction may also be used in polymer end-group analysis, polymer oxidation and degradation reaction analysis and inter-molecular analysis.

Below is the infrared spectra of traditional bis (2-ethylhexyl) phthalate (DEHP) plasticized rigid PVC and PVC materials used in medical infusion equipment.



#### 5.4 Polymer materials in ophthalmology

Contact lenses are the most common polymer product in ophthalmology. The basic requirements for this type of materials are: (1) excellent optical properties with a refractive index similar to cornea; (2) good wettability and oxygen permeability; (3) biologically inert, degradation resistant and not chemically reactive to the transfer area; (4) with certain mechanical strength for intensive processing and stain and precipitation prevention. The common used contact lens material includes poly- $\beta$ -hydroxy ethyl methacrylate, poly- $\beta$ -hydroxy ethyl methacrylate, Poly- $\beta$ -hydroxy ethyl methacrylate - methyl amyl acrylate and polymethyl methacrylate ester-Nvinyl pyrrolidone, etc. The artificial cornea can be prepared by silicon rubber, poly methyl

acrylate, poly-casein or other thin films. The main body of the artificial lens can be made of polymethacrylate. The researchers have attached increasingly great importance to the qualitative analysis of polymer materials for this kind of medical equipments. As explicitly specified in YY0477-2004 "Orthokeratology Using Gas Permeable Rigid Contact Lens", infrared spectrum analysis is adopted to determine the components of the lens materials. The following drawing is the infrared spectrum analysis of this material: point 2961cm-1 is the methyl characteristic peak of methyl acrylate; points 1104 cm-1 and 1046 cm-1 are characteristic absorption peaks of siloxane, points 1730 cm-1,1227 cm-1 and 1199 cm-1 are ester peaks of methyl acrylate; points 893 cm-1 and 7556 cm-1 are the structure characteristic peak of fluoro-alkylated methyl acrylate.

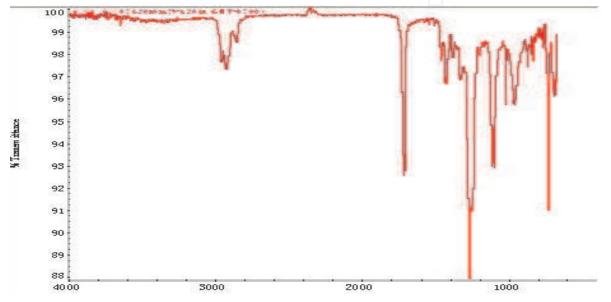


Fig. 6. Infrared spectrogram of PVC

5.5 The innovation of instrument performance and the development of computer application technology provide possibility for combined use of the previous stand-alone analysis instruments. The combined use of various types of instruments has greatly improved the accuracy and reliability of the analysis and testing results. With combination use of thermogravimetric analysis and IR spectrum and other analytical methods in recent years, thermogravimetric analysis is increasingly playing an important role in study of thermal behavior in chemical materials. In comparison with traditional thermogravimetric analysis method, TGA-IR spectrum combined analysis can directly and accurately determine the various physical-chemical change during the heating proves and identify the chemical composition of decomposition or degradation products during the during the weight loss process. Thus, it has been a key experimental method in studying thermostability and thermal decomposition (degradation) process of various inorganic, organic and polymer materials and proves a promising prospect in respect of thermal performance analysis of the materials. As Fourier transform infrared spectrometer is of high noise-signal ration and high precision, it may detect the slight intensity change and frequency shift of the infrared bands in the sample before and after the heat treatment. Thus to provide structural differences of polymer film for three different thermal stages of high molecular polymer, from high-elastic state slow cooling, high-elastic state quenching to heat treatment below temperature Tg. The

study shows the conformation changes of PVC films with different thermal histories in heating process. Meanwhile, in FTIR measurement, the sample subjected to heat treatment below Tg temperature occurred sudden change of conformation in the temperature range corresponding to enthalpy absorption peak of differential scanning calorimetry (DSC).

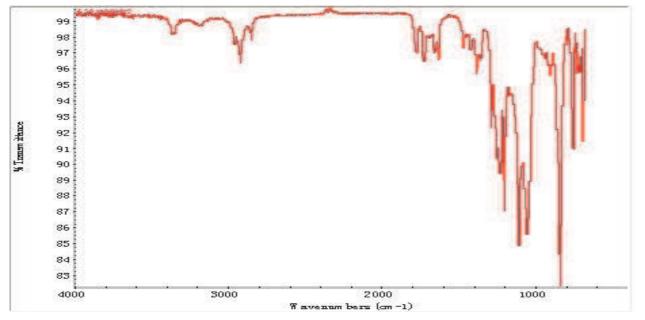


Fig. 7. Spectrum of Orthokeratology Using Gas Permeable Rigid Contact Lens

#### 6. Prospect

FTIR is becoming widely used in the field of medical polymer materials, especially for quantitative analysis of the material properties. At present, the study on application of infrared spectroscopic technology or combined application of IR spectrum with other technologies in polymer material, to be still growing. With rapid development of scientific technology, the research in IR spectrum is further deepened. IR spectrum is not only widely used in polymer materials but is also widely used in pharmaceuticals, foods and environmental science. The gradually improved infrared detection method may be used on vivo analysis of pathological tissue and greatly contribute to the rapid and accurate diagnosis of the diseases. Meanwhile, the disease mechanism and progression maybe clarified through analysis of infrared spectrogram of tissues or cells.

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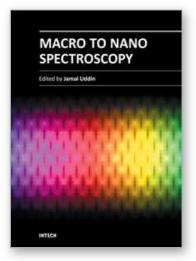
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In the last few decades, Spectroscopy and its application dramatically diverted science in the direction of brand new era. This book reports on recent progress in spectroscopic technologies, theory and applications of advanced spectroscopy. In this book, we (INTECH publisher, editor and authors) have invested a lot of effort to include 20 most advanced spectroscopy chapters. We would like to invite all spectroscopy scientists to read and share the knowledge and contents of this book. The textbook is written by international scientists with expertise in Chemistry, Biochemistry, Physics, Biology and Nanotechnology many of which are active in research. We hope that the textbook will enhance the knowledge of scientists in the complexities of some spectroscopic approaches; it will stimulate both professionals and students to dedicate part of their future research in understanding relevant mechanisms and applications of chemistry, physics and material sciences.

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