UNIVERSITI PUTRA MALAYSIA

PHASE BEHAVIOUR PHYSICAL PROPERTIES OF BATYL ALCOHOL

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Batyl alcohol (monoalkylether glycerine) acts as an emulsifier when used in emulsion products, such as cosmetics creams, lotions and ointments. It is chemically stable, highly purified and safe. Although batyl alcohol is widely used in cosmetic products, little is known about its phase behaviour and rheological properties in ternary systems. Its phase behaviour in ternary systems was therefore studied at 80°C, and observed under a polarising microscope.

In the ternary systems, lamellar and hexagonal areas were found in 90/10 and 100/0 mixtures of batyl alcohol (BA) and isopropyl myristate (IPM) and the percentage of water were from 9% - 44% w/w, respectively. They were identified by their patterns of maltese crosses and fan structures, respectively.

Both of them exhibited a viscoelastic network. Further addition of either medium chain triglycerides (MCT) or propylene glycol (PG) to the system resulted in isotropic and two-phase areas being formed instead of a liquid crystalline structure.

Using a combination of BA, IPM, MCT and water, an emulsion was developed. A ratio of 1:1 MCT:water was emulsified with 5% and 10% BA. A weak viscoelastic network was formed with 5% BA but without stearic acid (Emulsion S1). With stearic acid (Emulsion S2) a strong viscoelastic network was formed with the acid acting as a co-emulsifier. No network structure was found in the emulsion containing 10% BA (Emulsion S4) as it was stabilized by the right percentage of BA. The emulsifiers adsorbed at the MCT/water interface, reducing the droplet size and increasing the viscosity, while the rest formed liquid crystalline lamellar in the continuous phase to physically trap the droplets in the network. The conductivity measured revealed that oil-in-water emulsion can conduct electric and it also shows the oil droplets encapsulated by the emulsifier in S2.

Abstrak tesis yang dikemukakan kepada Senat Universiti Putra Malaysia
sebagai memenuhi keperluan untuk ijazah Master Sains

KELAKUAN FASA DAN CIRI-CIRI FIZIKAL BAGI BATIL ALKOHOL

Oleh

LIM CHAI SENG

Jun 2004

Pengerusi: **Profesor Anuar Kassim, Ph.D**

Fakulti: **Sains dan Pengajian Alam Sekitar**

Batil alkohol (monoalkileter gliserin), apabila digunakan dalam barangan emulsi seperti krim kosmetik, losyen dan salap, ia akan bertindak sebagai pengemulsi. Sebatian ini adalah stabil dari segi kimia, sangat tulen dan selamat digunakan. Walaupun batil alkohol digunakan secara meluas dalam barangan kosmetik, pengetahuan terhadap kelakuan fasa dan sifat reologi dalam sistem tiga fasa agak kurang. Kelakuan fasa dalam sistem tiga fasa telah dikaji pada 80°C serta dilihat malalui cahaya berpengutub dan disahkan dengan mikroskop berpengutub.

Dalam sistem tiga fasa, fasa lamelar dan heksagonal terdapat pada kombinasi 90/10 dan 100/0 batil alcohol (BA)/ isopropil miristat (IPM) dan peratus air adalah dari 9% - 44% w/w masing-masing dan mereka telah

diidentifikasi sebagai corak palang maltese dan taring masing-masing. Kedua-duanya menunjukkan jalinan hablur cecair yang bersifat viskoelastik. Isotropik dan kawasan dua fasa telah terbentuk dengan penambahan trigliserida rantai sederhana (MCT) dan propilena glikol (PG) kepada sistem ini.

Dengan campuran BA, IPM,MCT dan air, sistem emulsi telah dimajukan. Nisbah 1:1 bagi MCT dan air telah diemulsi dengan 5% dan 10% BA. Terdapat satu viskoelastik yang lemah telah terbentuk dalam sampel S1 dengan 5% BA tanpa asid stearik tetapi dengan kehadiran asid stearik dalam sampel S2, satu viskoelastik yang kuat telah terbentuk. Asid stearik bertindak sebagai pengemulsi bersama. Emulsi yang mengandungi 10% BA dalam S4 tidak terdapat sebarang viskoelastik. Sistem distabilkan dengan menggunakan peratusan BA yang betul. Pengemulsi menjerap pada antara muka MCT/air, mengurangkan saiz titisan, meningkatkan kelikatan, semasa yang lain membentuk lamelar hablur cecair dalam fasa terusan sehingga memerangkap titisan secara fizikal. Pengukuran kekonduksian menunjukkan emulsi minyak dalam air boleh mengkonduksi elektrik dan ia juga menunjukkan titisan minyak diperangkap oleh pengemulsi dalam sistem S2.

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LIST OF ABBREVATIONS

BA = Batyl Alcohol

IPM = Isopropyl Myristate

MCT = Medium Chain Triglyceride

PG = Propylene glycol

TEA = Triethanolamine

SA = Stearic Acid

CHAPTER 1

INTRODUCTION

1.1 Liquid Crystal

Otto Lehmann, a physicist, first coined the term *liquid crystal* to describe materials which share many of the properties of both the liquid and solid states. The first liquid crystalline material discovered was an organic substance related to cholesterol - cholesterol benzoate. It was actually first observed around 1850 by Heintz, a chemist working on natural fats, but only reported in 1888 by Friedrich Reinitzer, an Austrian botanist.

The meaning of "liquid crystal" has been enormously extended in the last two decades to encompass both the chemical and structural concepts. In general, it is accepted that liquid crystals represent a higher state of order than ordinary (isotropic) liquids. However, the delimitation from crystalline solid is less clear. Liquid crystals possess greater intermolecular and intramolecular mobility than classical solids, with many types having a lower degree of order than crystalline solids. However, there are several types of highly ordered smectic liquid crystals, which possess a three-dimensional order, and are therefore designated "crystal" phase types by Mori *et al.* (1997).

There are three commonly recognized states of matter - solid, liquid and gas. Solid may be either crystalline or amorphous. Crystalline solids have a regular arrangement of their molecules over a large distance compared to their molecular dimensions, or a long-range order. When a crystalline solid is heated, it transforms into an isotropic liquid at its melting point. The isotropic liquid does not have any long-range order. Conversely, on cooling, the isotropic liquid is transformed into a crystalline solid (Ekwall, 1974).

For years after their discovery, liquid crystals remained a scientific curiosity. They were studied by scientists, who thought they had learnt everything about them by the end of the Second World War. The past decade though has witnessed new impetus in liquid crystal research with specific applications in such diverse areas as medicine, biology, chemistry, physics, space science, mathematics and engineering (Westerman, 1993).

Liquid crystal is a material that can transform from the solid to liquid state and *vice versa* with an intermediate phase in between – the mesomorphase. Thus, liquid crystal is similar to a liquid–free flow due to the absence of positional order. On the other hand, liquid crystal also resembles a crystalline solid because it maintains some orientation. Basically, liquid crystal is divided into *lyotropic* and *thermotropic.* A lyotropic liquid crystal is formed when a surfactant is mixed with a solvent whereas a thermotropic liquid crystal is formed over a certain temperature range (Ekwall, 1974).

1.1.1 Lyotropic Liquid Crystal

The word “lyotropic” means “solvent-induced”, which starts with molecules that are amphiphilic. Amphiphilic molecules are composed of two different parts - a nonpolar, or hydrophobic, hydrocarbon tail insoluble in water, and a polar or hydrophilic head soluble in water. Some amphiphilic molecules that form lyotropic liquid crystals under controlled conditions are soaps, bile salts and phospholipids (Collings, 1990). When these compounds are dissolved in water, they can form spherical aggregates such as micelles, or vesicles, or cylindrical structures such as a bilayer. These structures float freely in the water but retain their orientation and positional order.

It has long been recognized that liquid crystalline phases form a water miscible surfactant, which, when dissolved in water above a well-defined concentration, form aggregates (micelles). As the surfactant concentration increases, the physical characteristics of the solution will change the nature of the aggregated solute. These aggregates are the building blocks of the liquid crystal phases that occur at higher concentration.

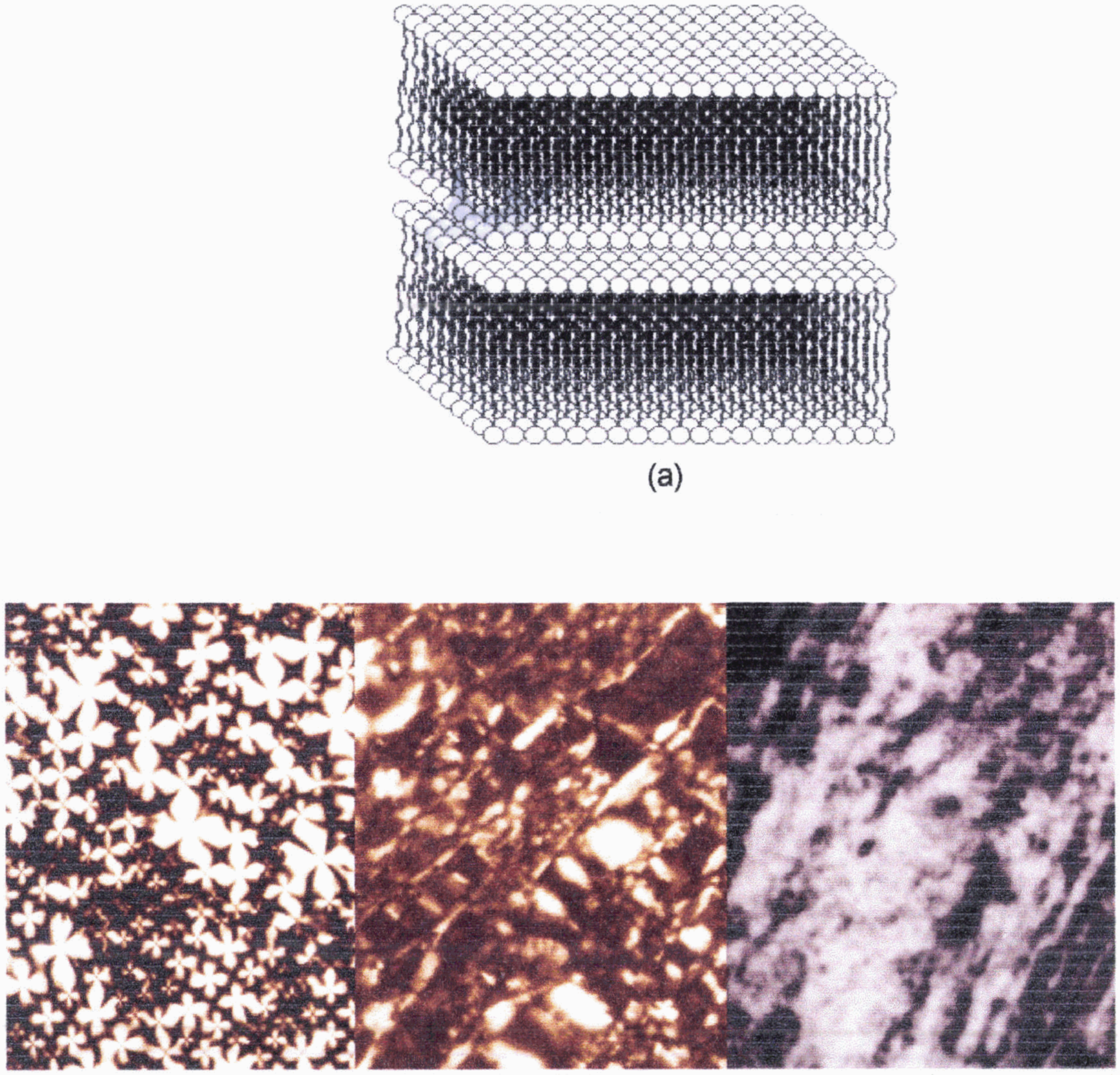
1.1.2 Classification of Lyotropic Liquid Crystal

There are six classes of lyotropic liquid crystal - lamellar, hexagonal, cubic, nematic, gel and intermediate phases. All of these have been recognized for many years except the intermediate phase. However, for simplicity, only the two major types are discussed - lamellar and hexagonal. Furthermore, different lamellar liquid crystals are formed from different combinations of interlayer spacings.

1.1.3 Lamellar Phase

The most common lyotropic liquid crystal form in a surfactant system is the lamellar phase (Figure 1.1), also known as the neat phase. The lamellar structure is the most extensive liquid crystal phase studied as it has only a simple one-dimensional order. In this phase, the surfactant molecules are arranged in bilayers, separated by water layers.

The surfactant in the bilayer is arranged such that the hydrophobic groups of the surfactant molecules are located in the center of the bilayer. The hydrophilic groups are therefore attached to the solvent layer. Viewed under a polarising microscope, the liquid crystal has three optical patterns – Maltese crosses, oily streaks and striation (Figure 1.1b). The thickness of the bilayer structure is dependent on the water content - increasing the water content will increase the area per polar head group of the occupied interface (Ekwall, 1975; Small, 1988).



(a)

(i) (ii) (iii)

(b)

Figure 1.1: Lamellar liquid crystal (a) Schematic structure, and (b) Typical patterns in it: i) Maltese crosses, ii) oily streaks, and iii) striation.