

**SOCIETY OF COSMETIC CHEMISTS**

**SCC**

Dedicated to the Advancement of Cosmetic Science

# Oil Soluble Silicones

Southeast Chapter

March 19, 2015



# Background

- **Silicone compounds have been known since 1860, but were of little commercial interest until the 1940's.**

# Background

- **Silicone compounds have been known since 1860, but were of little commercial interest until the 1940's.**

# Background

- **Over the years, silicone compounds have received growing acceptance in many personal care applications. In fact it has been said that four of ten new personal care products introduced in the 1990's have silicone in them.**

# Quartz



# Silicon







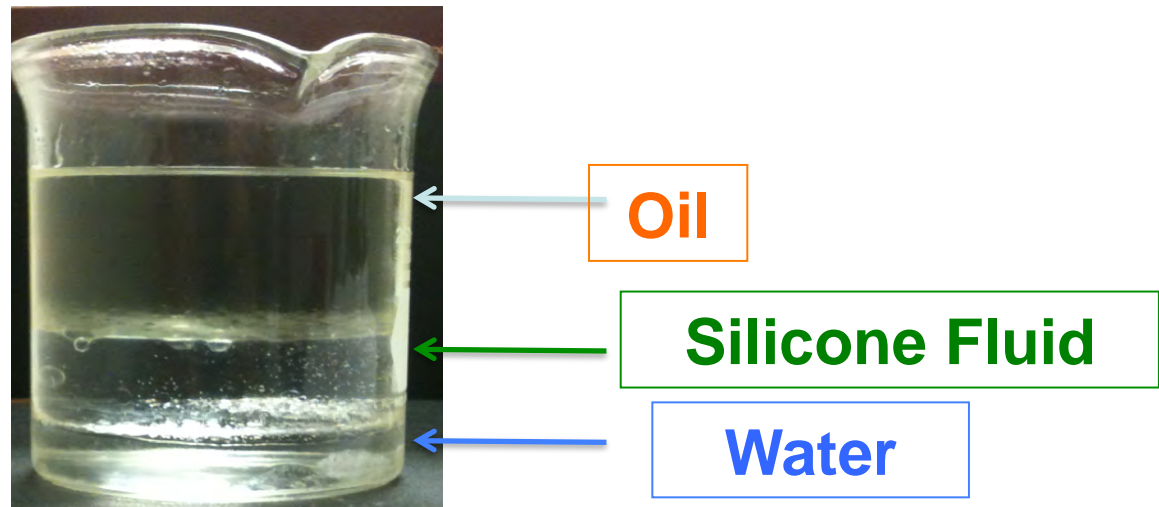


Why Silicone?



# Solubility

- Materials can be defined can be defined by solubility:
  - **Hydrophilic (Water-loving) / Hydrophobic (Water-hating)**
  - **Oleophilic (Oil-loving) / Oleophobic (Oil-hating)**
  - **Siliphilic (Silicone-loving) / Siliphobic (Silicone-hating)**



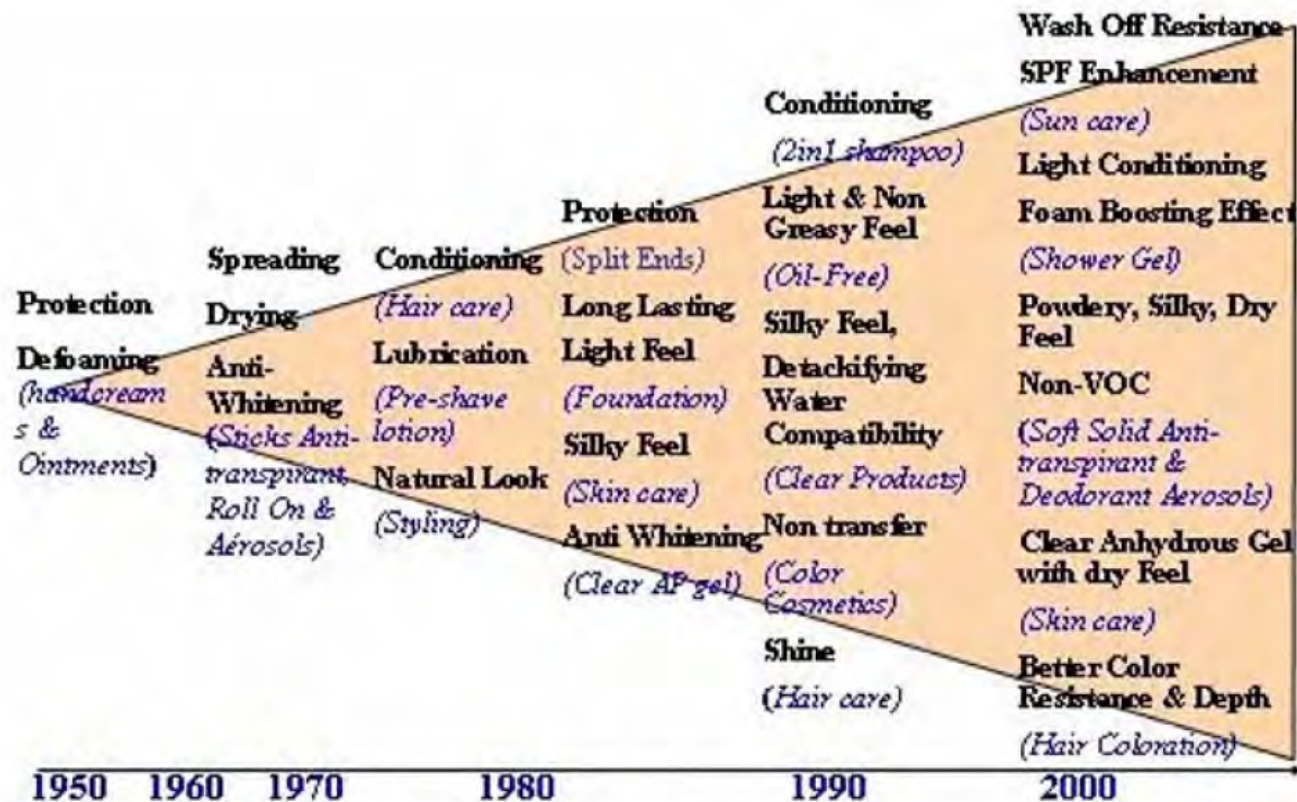
# Surface Tension

- Water 72 dynes/cm
- Oil 32 dynes/cm
- Silicone 25 dynes/cm
- Fluoro 15 dynes/cm

# Silicone Properties

- Surface Tension Reduction
- Skin Feel
- Spread
- Film Formation
- Dry Feel

# Silicone Applications



# Amphiphilic Surfactants

- Amphiphile is from the Greek used to describe a chemical compound possessing both hydrophilic and lipophilic properties.
- Such a compound is called amphiphilic or amphipathic.



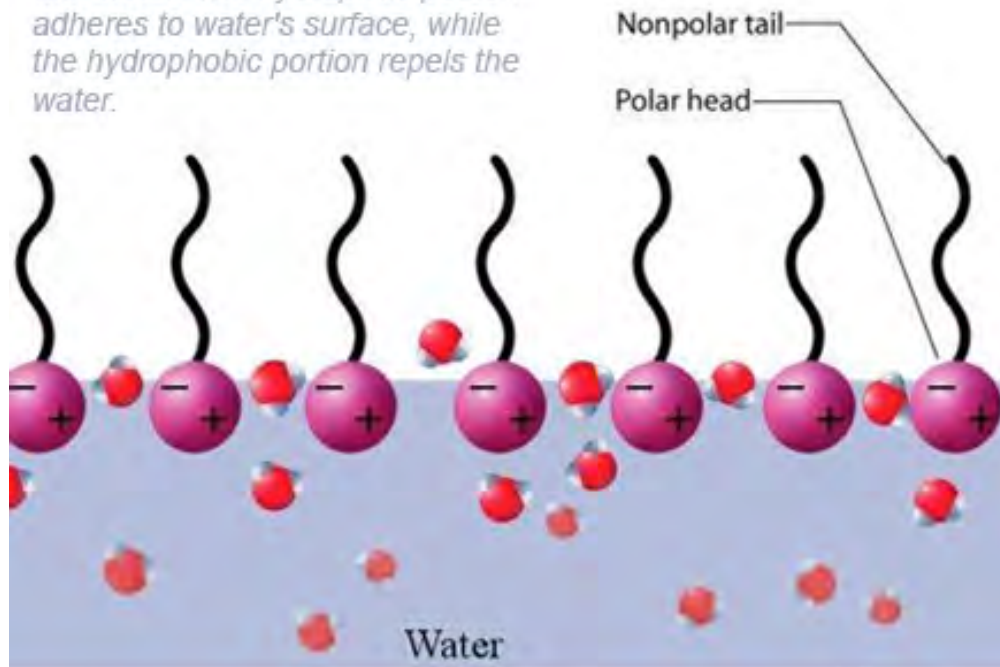
- We understand that despite the fact surfactants in water are SOLUBLE ( clear), we accept they are surface active.



- We also understand that surfactants lower water's surface tension from around 72 dynes/cm to around 32 dynes/cm.

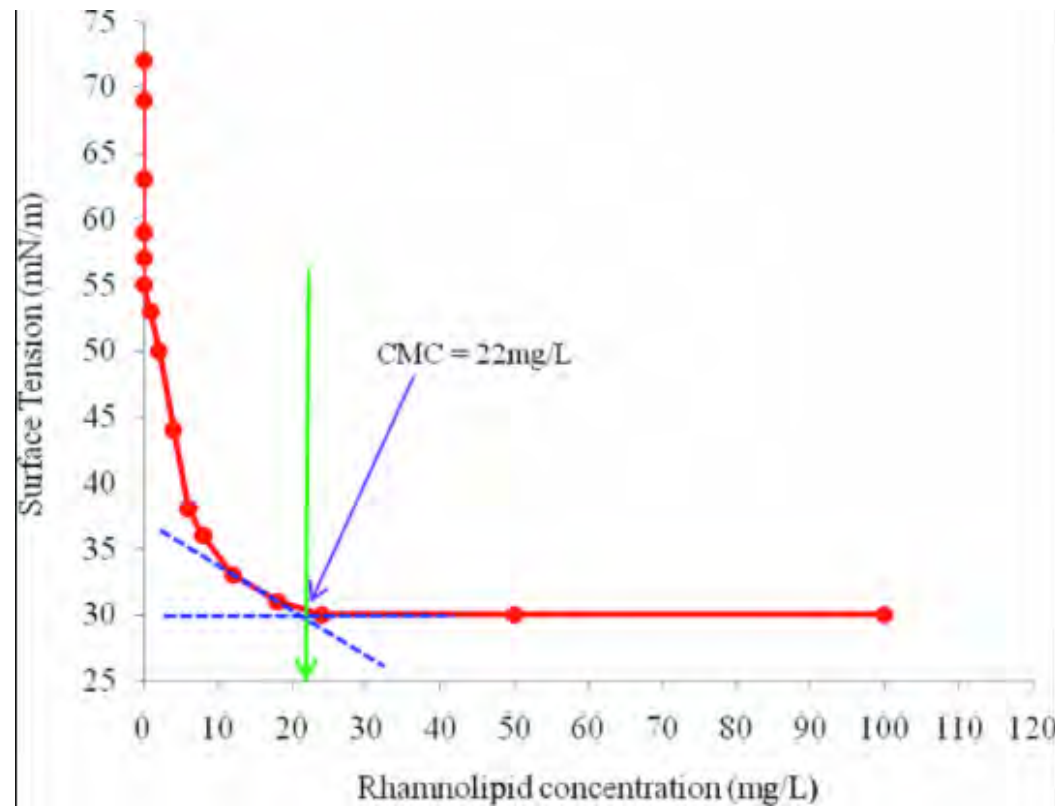
# Surfactants

*Here, a surfactant is shown binding with water. The hydrophilic portion adheres to water's surface, while the hydrophobic portion repels the water.*



We all understand oil based surfactants 16

# CMC Data



- But what about other insoluble phases?



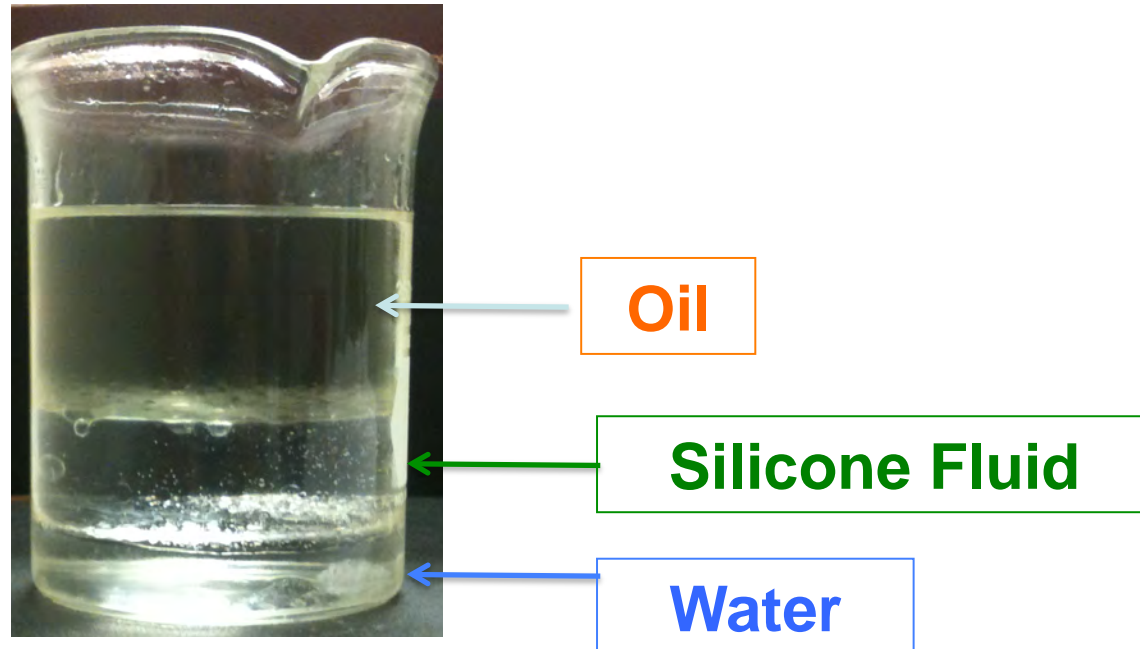
# Groups that are insoluble in each other

- Oil Phases
- Water Phases
- Silicone Phases
- Fluoro Phases



# Solubility

- Compounds can be defined as the following:
  - **Hydrophilic (Water-loving) / Hydrophobic (Water-hating)**
  - **Oleophilic (Oil-loving) / Oleophobic (Oil-hating)**
  - **Siliphilic (Silicone-loving) / Siliphobic (Silicone-hating)**



# Amphiphilic Compounds

- New Definition:
- Amphiphilic materials have two or more groups in the same molecule that in pure form are insoluble in each other.



# Oil Soluble Amphiphilic Compounds



## Oil Soluble Silicone:

1. Lower Surface Tension
2. Form Gels
3. Change Aesthetics
4. Minimize Syneresis

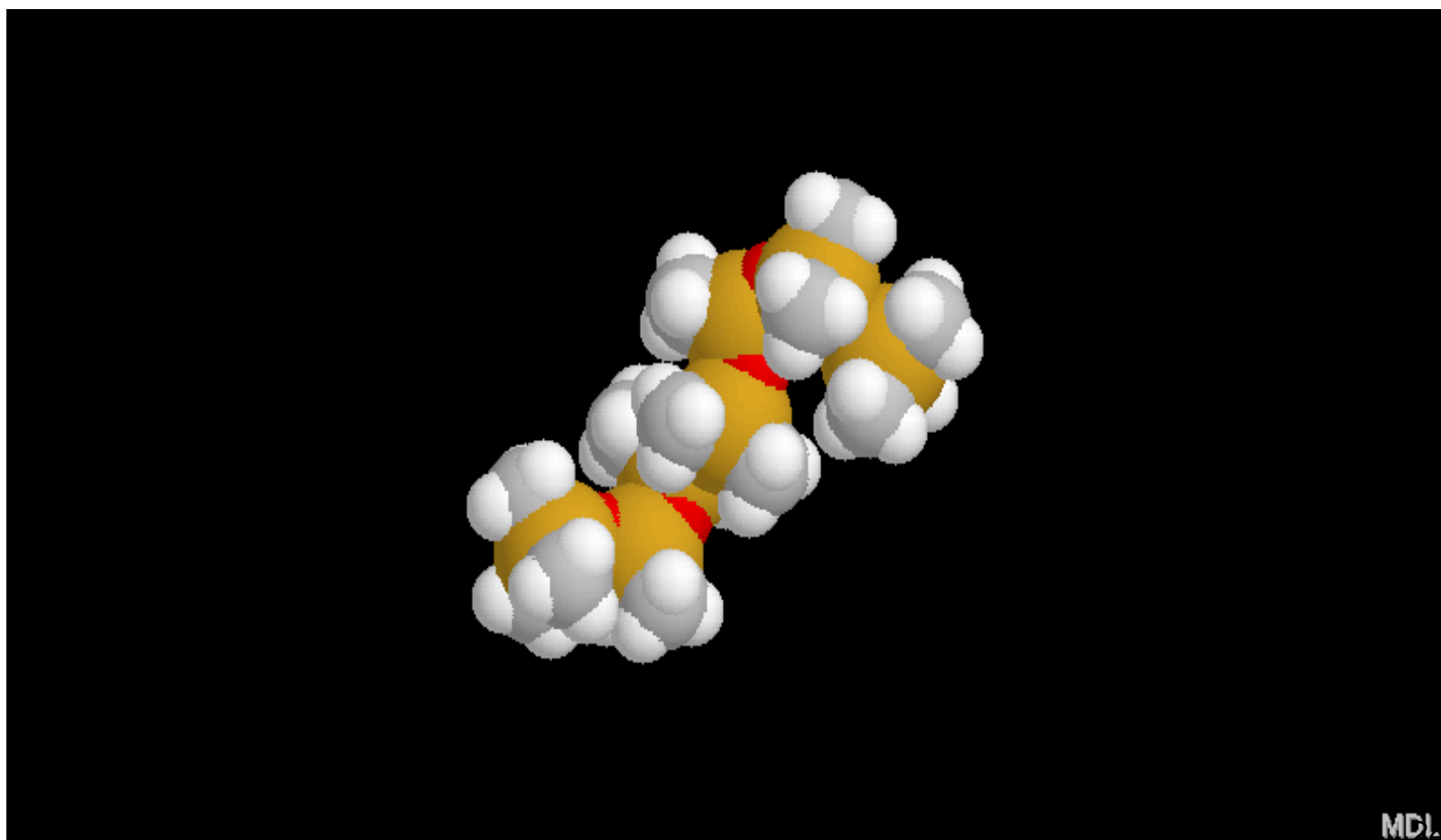
Contraction of a gel, causing separation of liquid from it





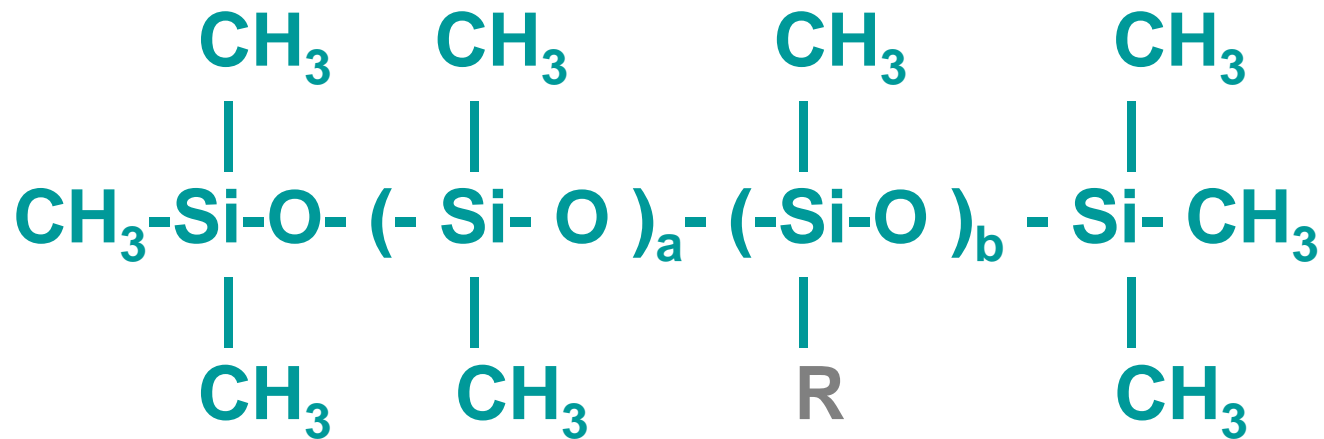


Why?





# Alkyl Dimethicone



R is alkyl





# Silicone Waxes

**The length of the alkyl chain controls the melt point of the wax.**

**Waxes based upon alkyl groups having between 12 and 16 carbon units are liquids at room temperature.**

**At carbon lengths of 18 and above products become solid and the melt point increases as the carbon length goes up.**



# Silicone Waxes

**The length of the alkyl chain controls the melt point of the wax.**

**Waxes based upon alkyl groups having between 12 and 16 carbon units are liquids at room temperature.**

**At carbon lengths of 18 and above products become solid and the melt point increases as the carbon length goes up.**

**The length of the silicone controls the hardness of the wax.**

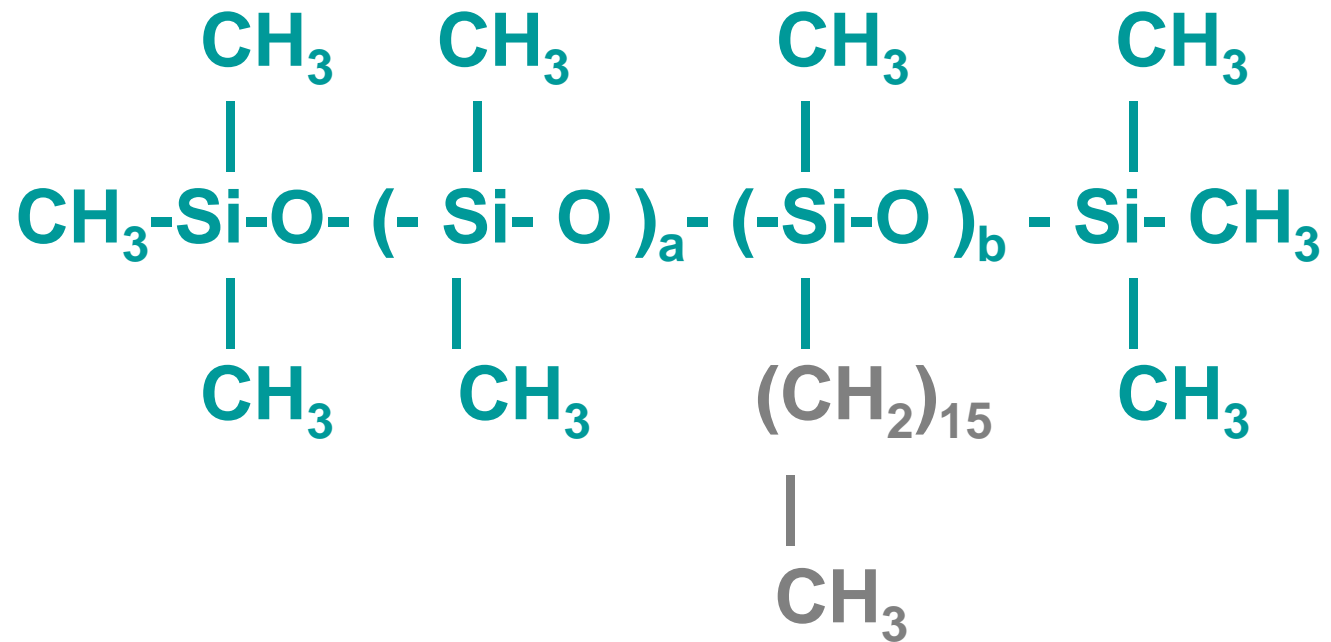
# Why Alkyl Dimethicone?

- liquid alkyl dimethicone compounds lower surface tension;
- and
- provide aesthetics due to uniform coverage.



# Alkyl Dimethicone

- Silwax B-116
- INCI: Cetyl Dimethicone
- Viscosity 25 cps
- Soluble in esters, triglycerides, and other oils.
- Feel Modifier,
- Surface Tension Reduction





# Alkyl Dimethicone

- Silwax B-116
- Improves spread by lowering surface tension.
- Makes oils feel more Siliphilic (silicone like).
- Add silicone feel.



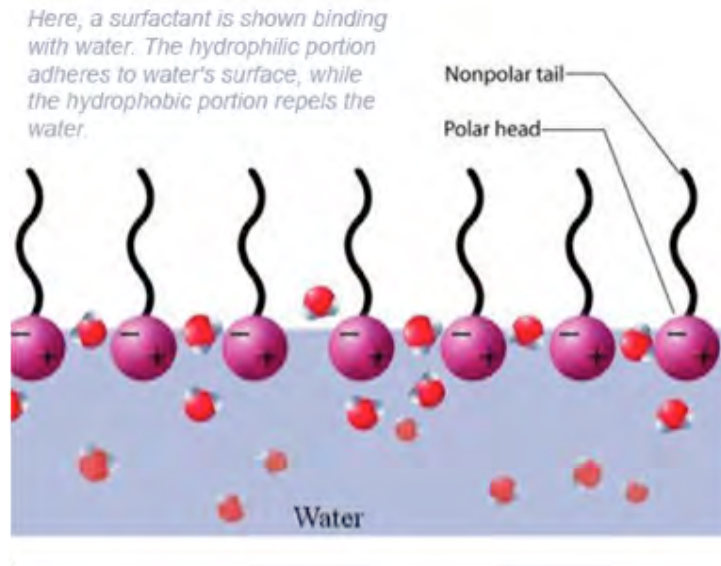
Not all “CMC” graph’s are as clean.

Therefore we measure to a fixed surface tension

**RF<sub>50</sub> = the concentration of silicone surfactant added to reduce the surface tension to 25 dynes/cm.**



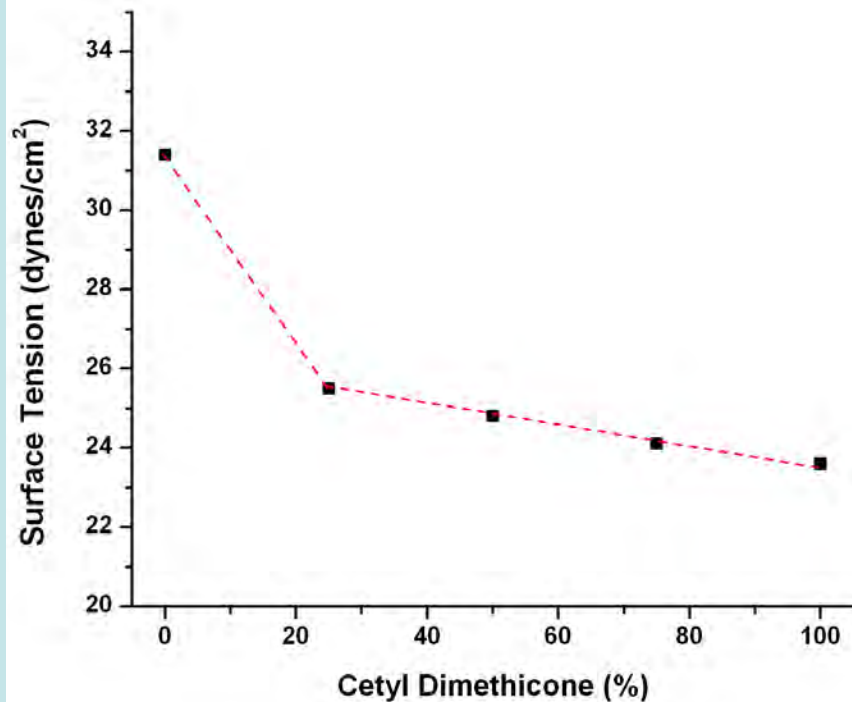
# Surface Tension Reduction



This occurs at low concentration as shown to the left for water based systems.



# Cetyl Dimethicone in Soybean Oil

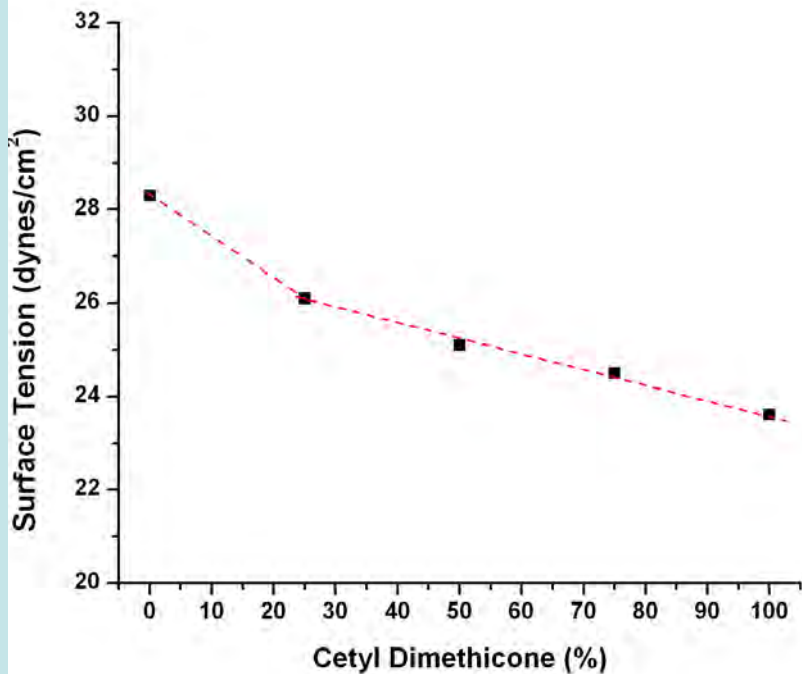


**RF<sub>50</sub> = the concentration of silicone surfactant added to reduce the surface tension to 25 dynes/cm.**

Soybean Oil (wt %)	Cetyl Dimethicone (wt %)	Surface Tension (Dynes/cm)
100	0	31.4
75	25	25.5
50	50	24.8
25	75	24.1
0	100	23.6



# Cetyl Dimethicone in Mineral Oil



**RF<sub>50</sub> = the concentration of silicone surfactant added to reduce the surface tension to 25 dynes/cm.**

**RF<sub>50</sub> is a measure of efficiency**

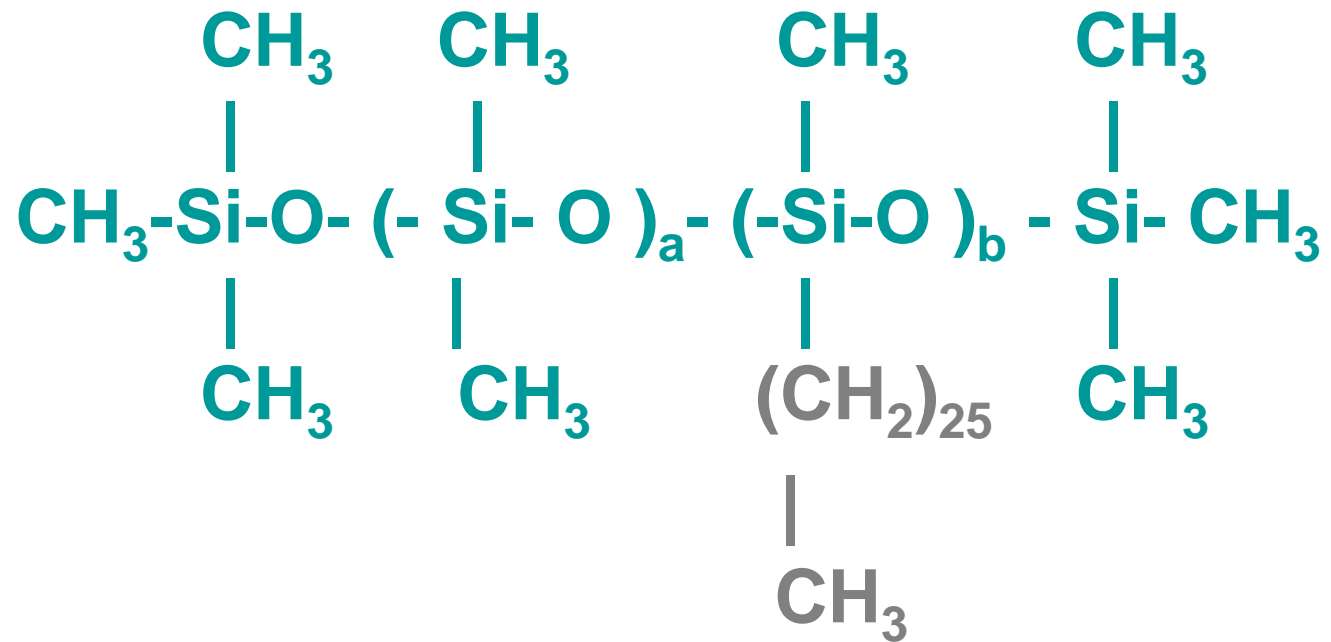
Mineral Oil (wt %)	Cetyl Dimethicone (wt %)	Surface Tension (Dynes/cm)
100	0	28.3
75	25	26.1
50	50	25.1
25	75	24.5
0	100	23.6



# Alkyl Dimethicone

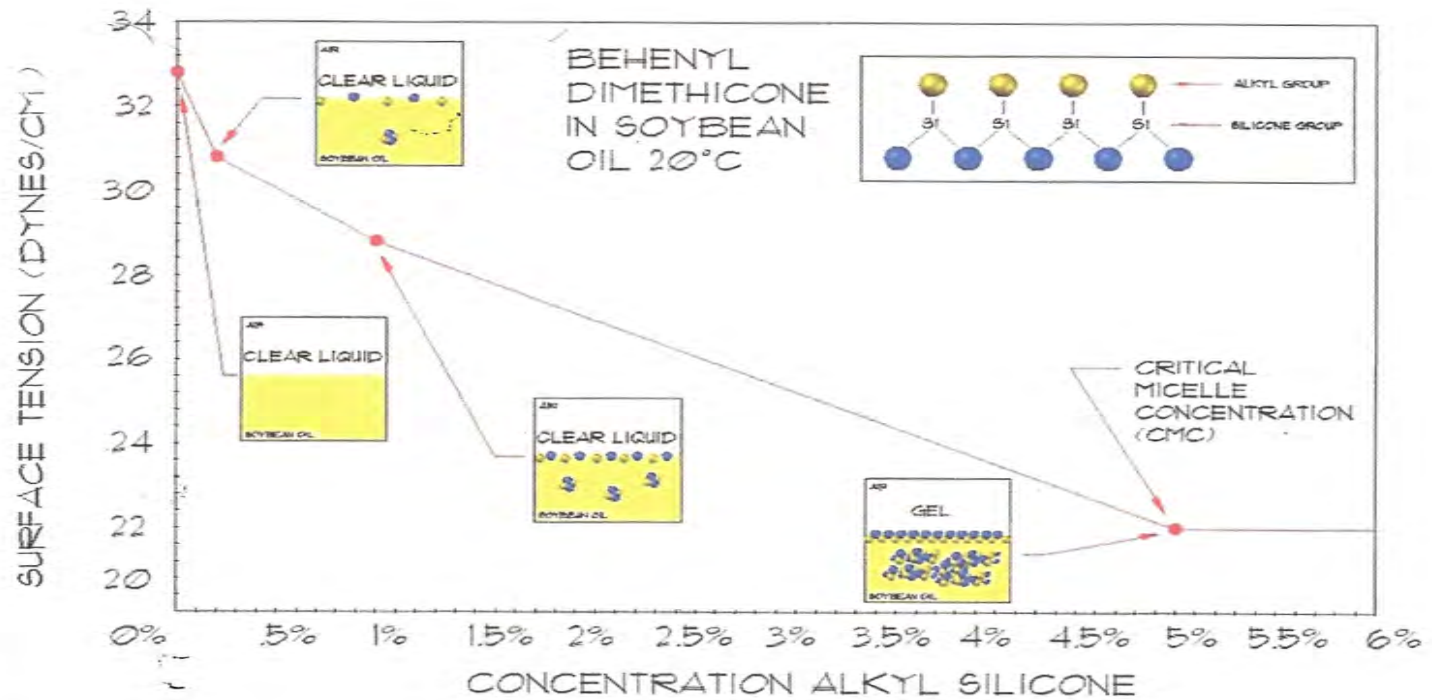
## Silwax D-226

- INCI Ceretyl Dimethicone
- Melt Point: 47°C
- Soluble in esters, triglycerides, and other oils





# Surface Tension Reduction

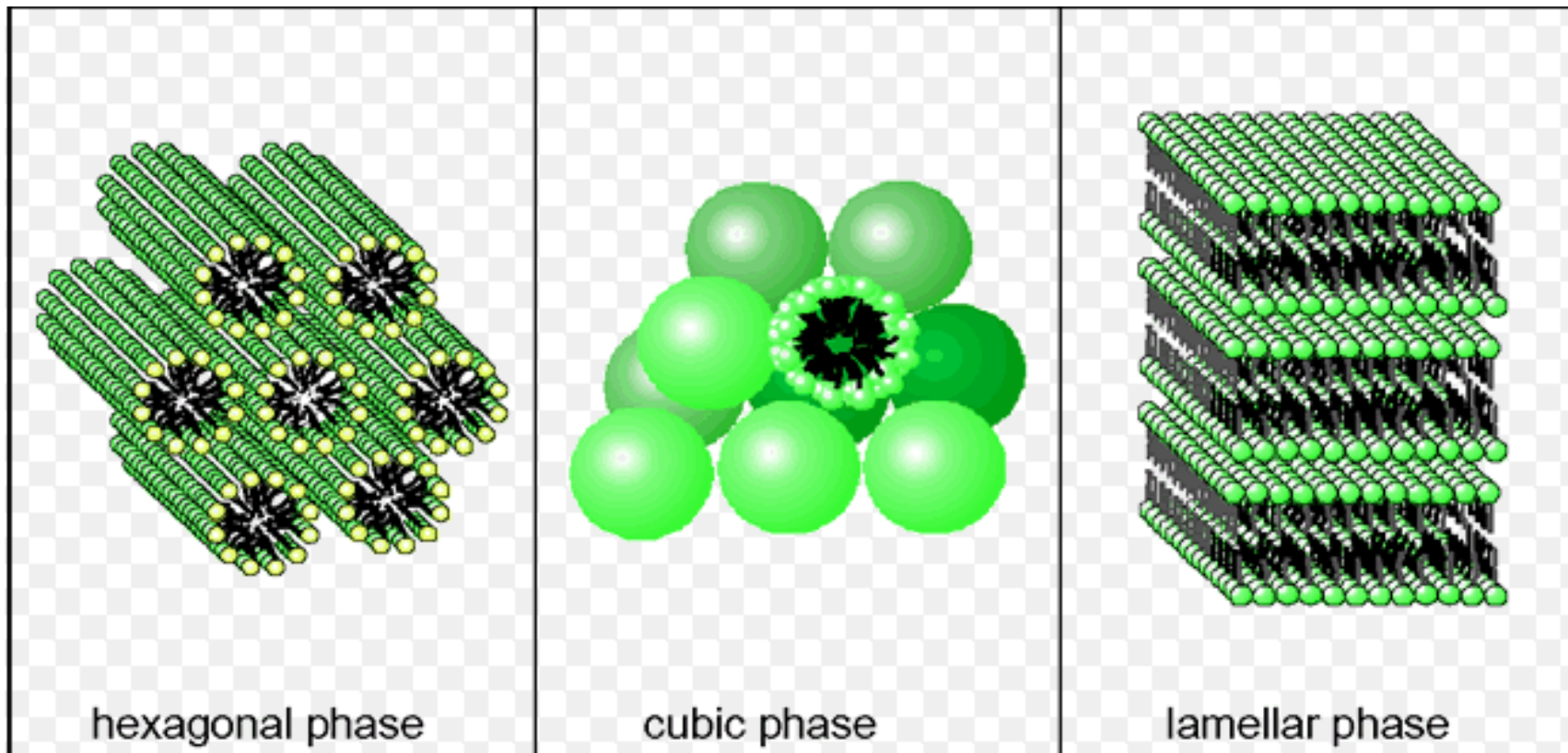


## Select RF50 and Cosmetic Properties

<b>Material</b>	<b>RF-50</b>	<b>Feel</b>	<b>Cushion</b>	<b>Play Time</b>
Cetyl Dimethicone	5%	Light	Moderate	Moderate
Ethyl Methicone	0.2%	Dry	None	Very low



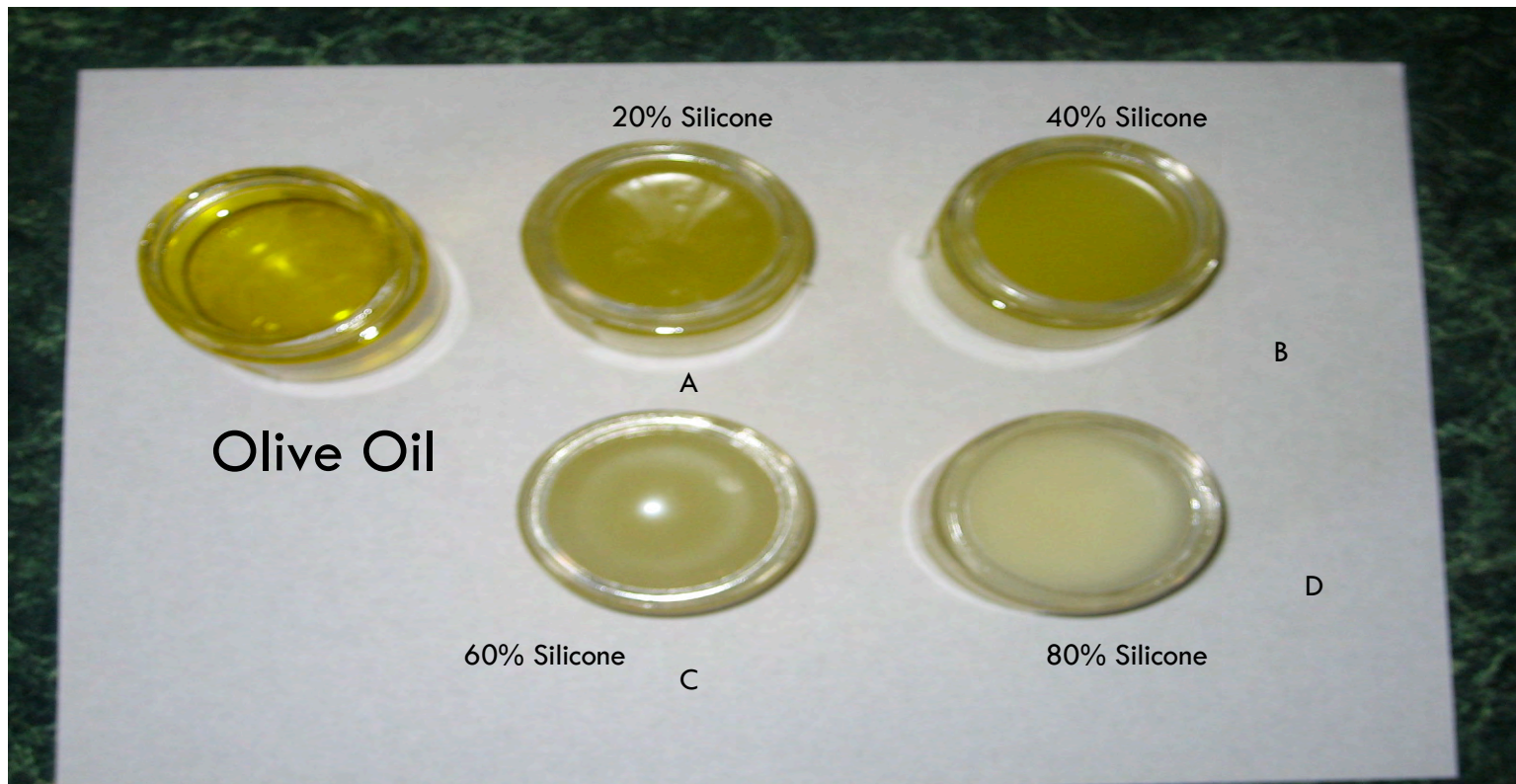
# What about Structured Compositions





# Behenyl Dimethicone

Gellation of Olive Oil ( 5% Additive)





# Critical Gel Concentration (CGC)

- The minimum concentration needed to make a system gel.

Silicone Gels 50 cst Fluid



Percent Wax Added

0%

10%



20%

30%

40%

**Critical Gel Concentration**



What about complex aesthetics?

**MULTI ALKYL DIMETHICONE**



## Multinomial Alkyl Silicones

- **Multi-domain systems have become very attractive.**
- **In general, two or more polymers can be blended to form a wide variety of random or structured morphologies in order to obtain materials which combine the characteristics of both components.<sup>1</sup>**
- **This is very difficult to achieve through simple blending.**
  - **Most polymers are thermodynamically immiscible and form heterogeneous (multiphase) systems.**
  - **Weak interactions between the two phases leads to poor overall properties.**





# Morphology of Block Copolymers

- Block copolymers are known to undergo microphase separation and form various phase morphologies.
- Solid alkyl chains will form microdomains.
  - This method produces a wide variety of products that can cover a full spectrum of hard/soft gels.

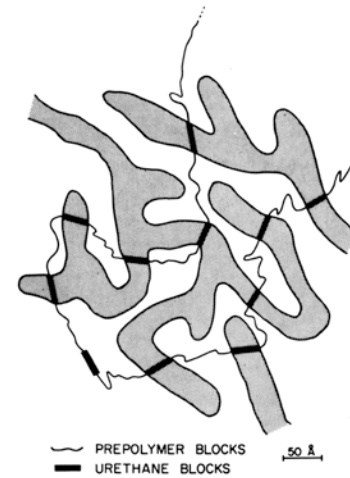
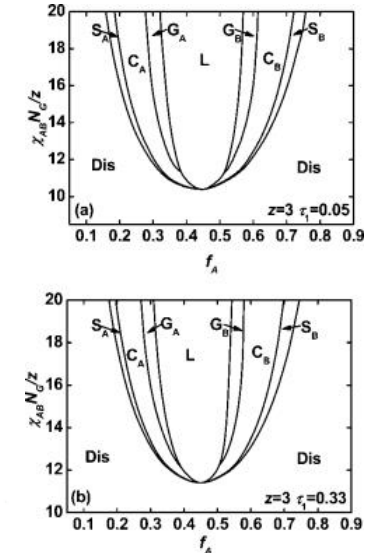
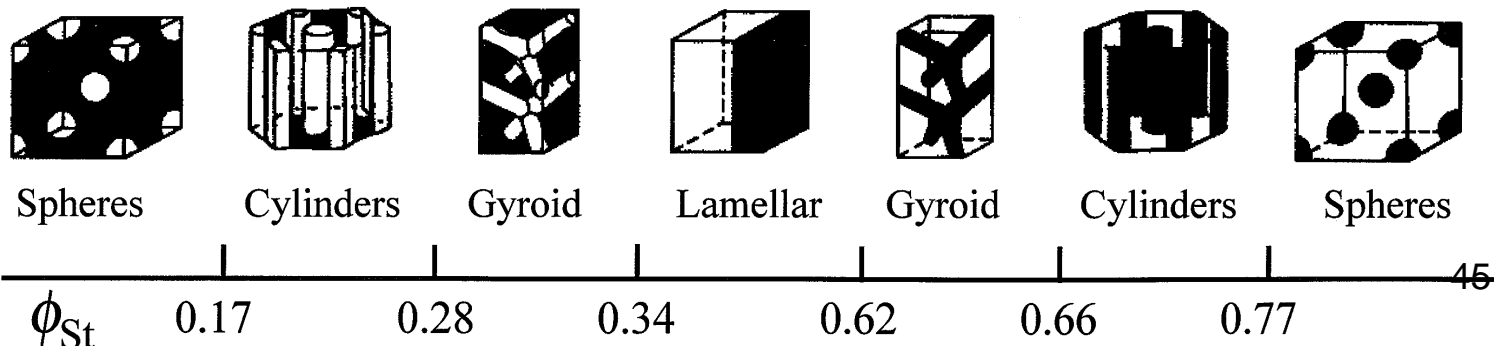


Figure 2. Representation of domain structures in a segmented copolymer

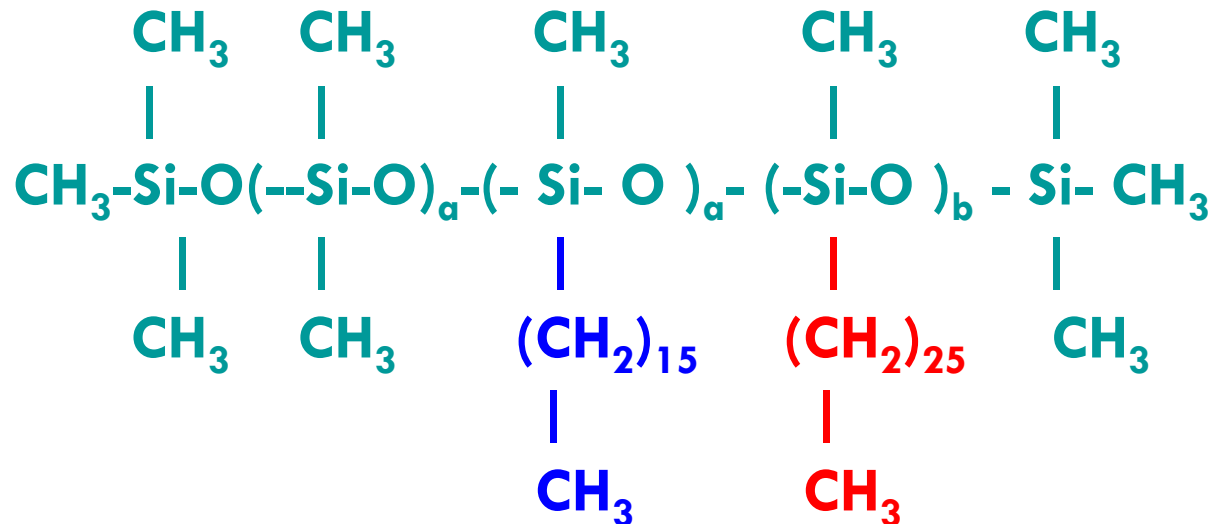


In Multiphase Polymers, Advances in Chemistry; American Chemical Society.



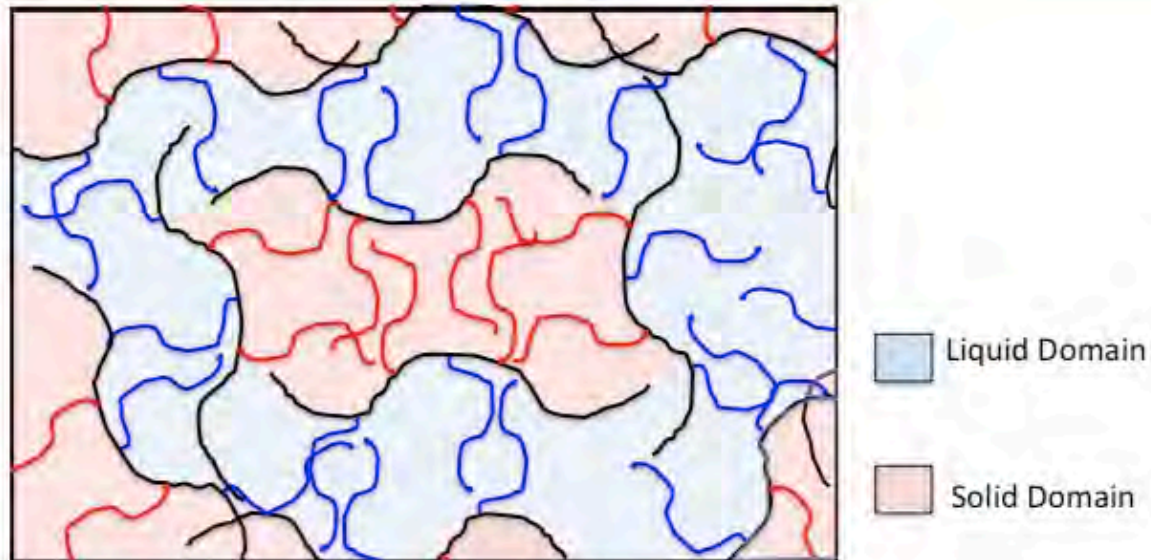


## Multi-domain Alkyl Dimethicone



- **Contain two different alkyl chain on the same silicone backbone**
  - One alkyl group is a short **LIQUID** carbon chain
  - One alkyl group is a longer **SOLID** carbon chain
- **These systems can self-assemble into organized networks, which can drastically change the properties of the polymer.**
  - **Rheology**
  - **Aesthetics**

# Morphology of Block Copolymers

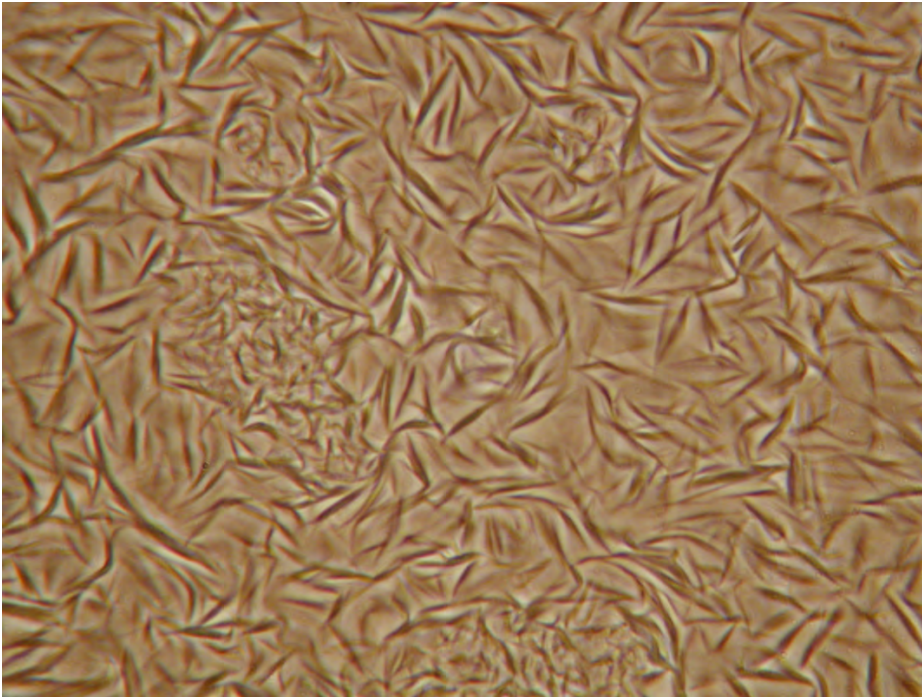


- As the polymer chains move past one another, the solid domains start to organize into small domains.
- After the solid side chains start to organize, the liquid domains are confined into the area around the solid domain.

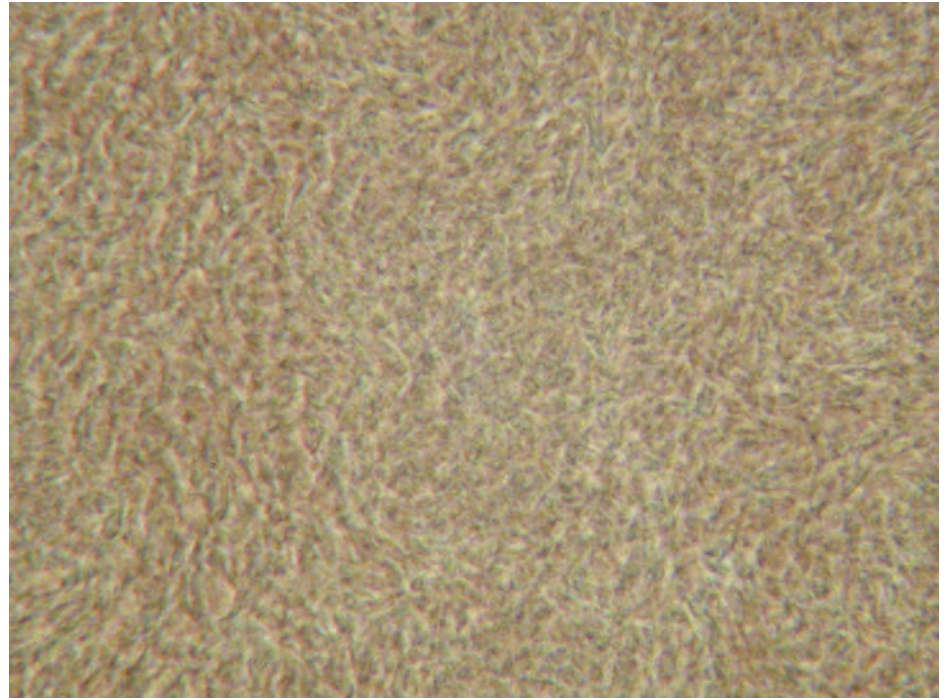




# Phase Contrast Microscopic Images



Multi-Domain



Polymer Blend



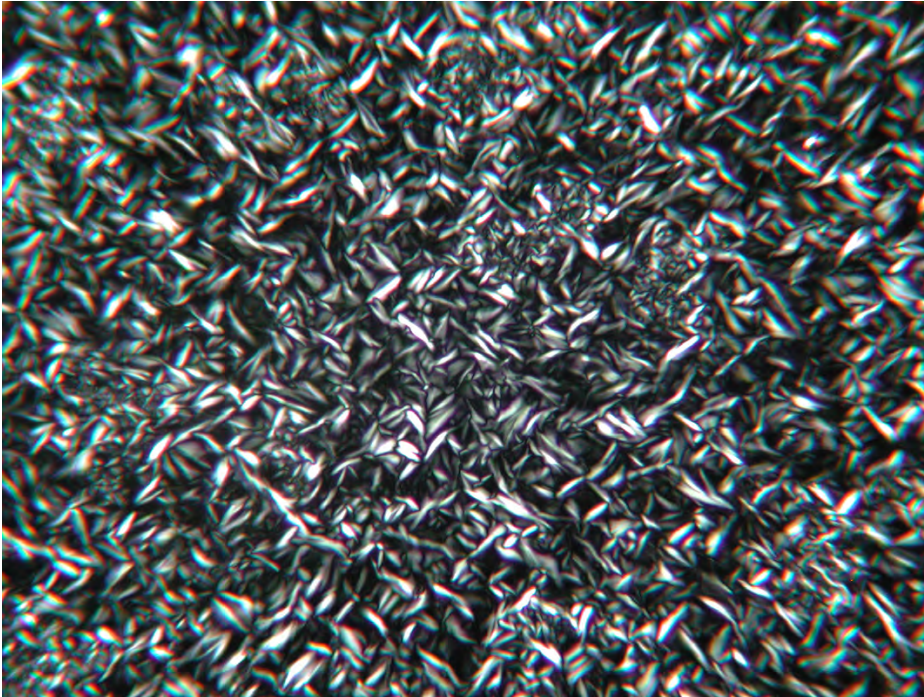
## Phase Contrast Microscopic Image of the Multi-Domain



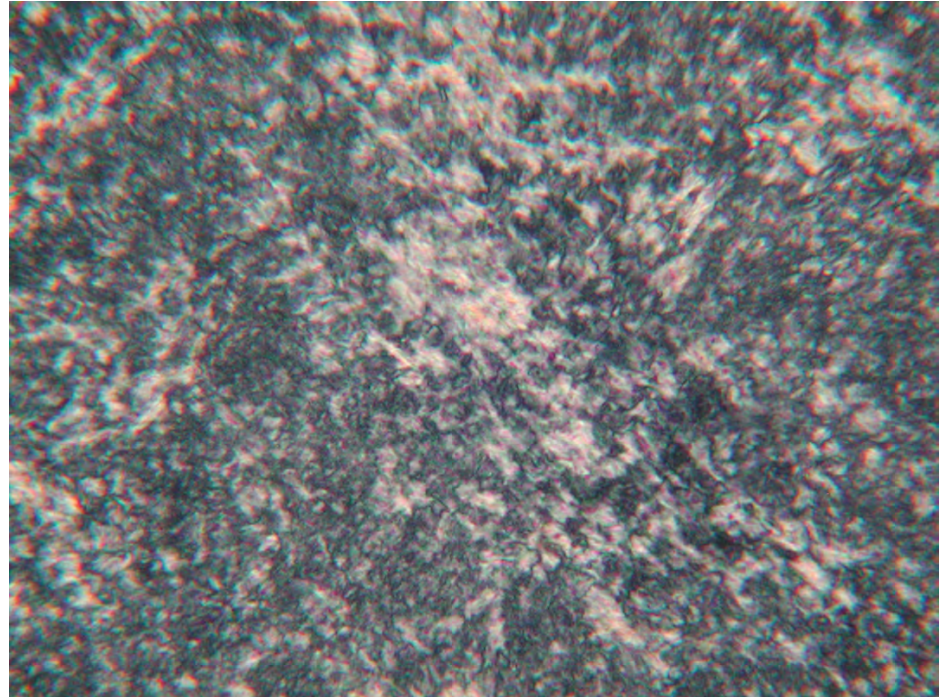




# Polarized Light Microscopic Images



Multi-domain

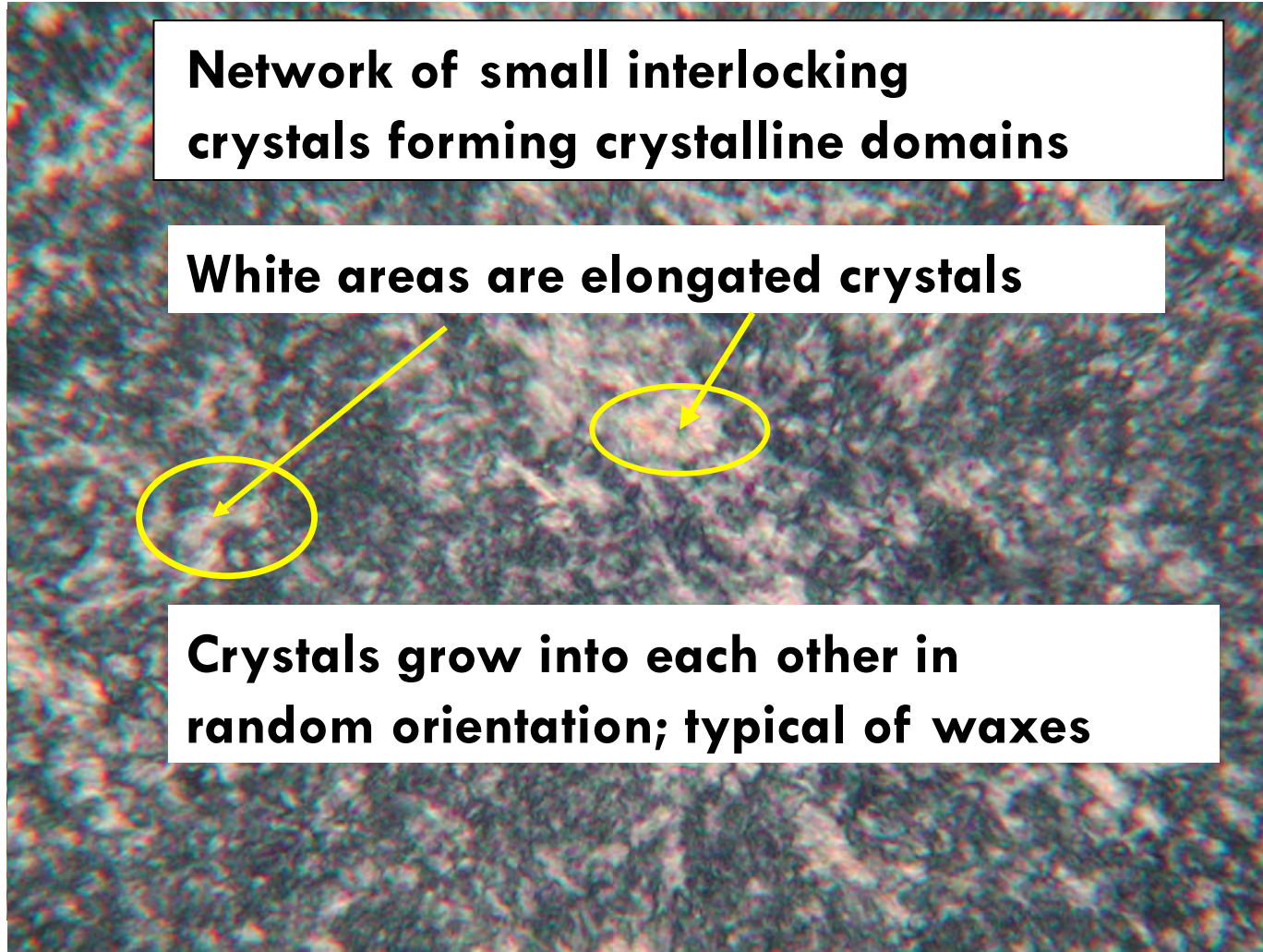


Polymer Blend





## Polarized Light Microscopic Image (Polymer Blend)





## Polarized Light Microscopic Image (Multi-domain)

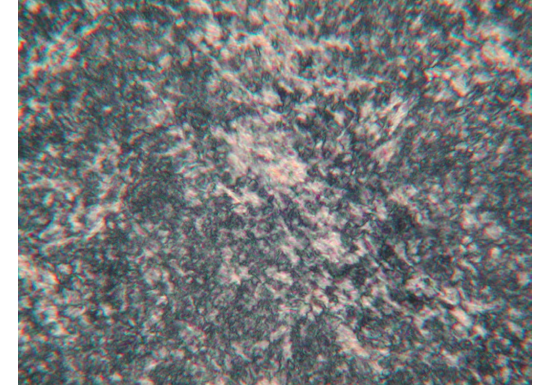
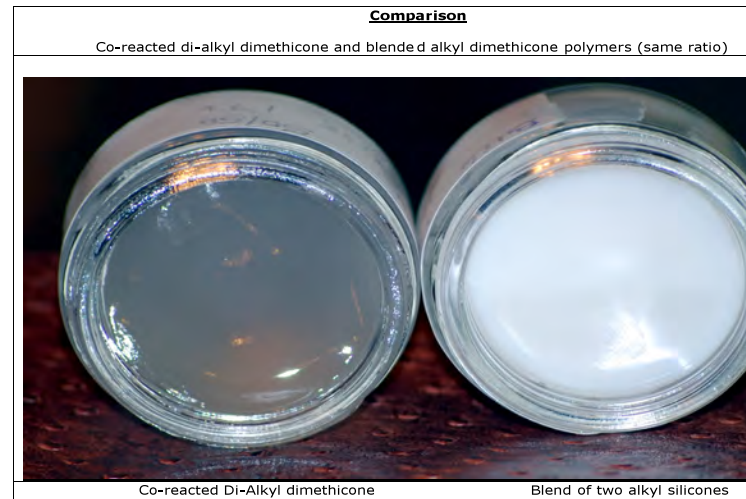
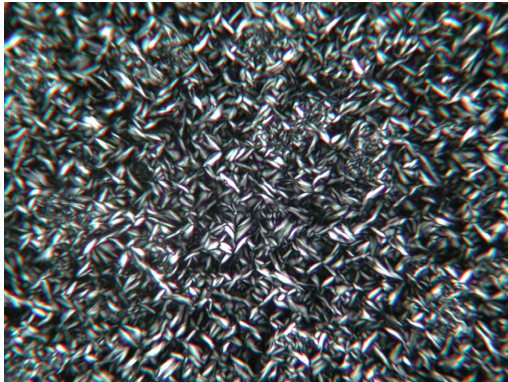
**Gel is a two phase liquid crystal system  
Solid Phase & Liquid Phase  
(surrounding the crystals)**

**Crystal arrangement is random and  
doesn't interlock as in the wax**





# Polarized Light Microscopic Images



## Multi-domain

- Melt Range = 34 – 38 °C
- Multi-domain
  - translucent gel
  - flows under pressure
- It is composed of two phases.
- The solid phase is crystalline and the relatively large, elongated crystals.
- Liquid crystals

## Polymer Blend

- Melt Point = 56 °C
- Polymer Blend
  - opaque
  - waxy
  - white
  - crystalline solid at room temperature.
- Ordinary Crystals



# Silwax D-221M

- **SILWAX® D221M** is one of a patent pending family of solid alkyl silicone, having different alkyl chains present on the same molecule. The result is a wider melting point product (34-37°C), and more importantly a very soft glossy feel on the skin.
- The product has been described as transient petrolatum, providing cushion that rapidly disappears to leave high gloss and no tack.
- INCI Cetyl hexacosyl dimethicone



# Formulations

- The ability to alter the feel of alkyl silicones by altering the ratio of the alkyl groups to each other, the ratio of silicone component, and the overall molecular weight allows the formulator to independently alter cushion and play time.
- The terms cushion and playtime are commonly used to describe the feel of ingredients and formulations on the skin. If one places a compound or formulation on the index finger and rubs it on the forearm, both cushion and playtime can be evaluated.





## Cushion

- The amount of compound that persists between the finger and forearm.
- That is the greater the “**distance**” between the finger and the forearm the greater the cushion.
- Honey has a great cushion. When tested in this manner there is a feeling of a great deal of material between finger and forearm.
- Water has little of no cushion. There is little “**distance**” between finger and forearm.



## Playtime

- Playtime refers to the **length of time** cushion persists.
- If the cushion is felt for a long period of time, the playtime is said to be **long**.
- If the cushion collapses rapidly the playtime is said to be **short**.



## Cosmetic Products

- In most compounds the cushion and playtime are directly related.
- Honey has both a high cushion and high playtime.
- There are however materials that have a good cushion but rapidly collapse having a low playtime.
- There are many applications in which a high level of **cushion**, and a **short playtime** are desired. These include **lipsticks, sun<sup>58</sup> products and many lotions.**



## **Multi Domain Silicone in Creams**

## MINDSPRING HAND CREAM +D221M

15-Apr-09

Project JW 3740 Client Ref  
 Formula Ref. 3915 \* 0 Formula Date 30/01/2009

*Creative Developments (Cosmetics) Ltd.*

*for creative cosmetic formulation & technical support*

[www.creative-developments.co.uk](http://www.creative-developments.co.uk)



## Siltech

Stage	Material	% w/w	Supplier	INCI Listing
<b>OIL PHASE</b>				
1	Decyl Oleate	5.000000	Purchased against approved specification	Decyl Oleate
2	Silwax D221M	2.000000	Siltech LLc	Behenyl Dimethicone
3	Cetearyl Alcohol	3.000000	Purchased to approved specification	Cetearyl Alcohol
4	Paraffin Wax	3.000000	Purchased to approved specification	Paraffin
5	Lasemul 92 N 40	2.000000	Industrial Quimica Lasem S.A.	Glyceryl Stearate
6	Amphisol K	2.500000	DSM Nutritional Products Europe Ltd	Potassium Cetyl Phosphate
<b>AQUEOUS PHASE</b>				
7	Water; Pure & Deionised	72.640000	Suitably deionised and treated	Aqua (Water)
8	Glycerine BP	5.000000	Purchased to approved specification	Glycerin
9	Sodium Lactate 60%	1.000000	PURAC biochem UK Ltd.	Sodium Lactate Aqua (Water)
10	Lactic Acid 88%	0.100000	PURAC biochem UK Ltd.	Lactic Acid Aqua (Water)
11	Lubrajel CG	3.000000	United-Guardian Inc	Glycerin Aqua (Water) Glyceryl Acrylate/Acrylic Acid Copolymer Propylene Glycol Methylparaben Propylparaben
12	Paratexin PPM	0.500000	S. Black Ltd	Phenoxyethanol Methylparaben Propylparaben
<b>COOLING CYCLE</b>				
13	Fragrance is AEC 38102 Complex	0.260000	A&E Connock Ltd.	Parfum (Fragrance)

**Mixing Instructions**

This is an ols to water mix at 70C.



## Alkyl dimethicone in Hand Cream

Hand Cream	3917 Hand Cream + Dimethicone	3915 Hand Cream +D221M	3916 Hand Cream + J221M
Appearance	Glossy white emulsion	Very smooth, glossy white emulsion	Smooth, glossy white emulsion
pH	4.7	4.7	4.7
Viscosity: T-Bar F Speed 1.5rpm	60% = 200K cps	57% = cps	70% = 233K cps
Application	Easiest to apply and rubbed in well	Easy to apply and rubbed in well	Easy to apply and rubbed in well
After feel	Nice after-feel	Acceptable	Best after feel; least sticky
Oil phase @ 70°C	Cloudy	Clear	Clear
Microscope	Small droplets widely dispersed in uneven emulsion.	Coarse droplets widely dispersed in uneven emulsion. Some evidence of liquid crystals	Very small droplets densely packed and evenly distributed. Some evidence of liquid crystals

All Creams were white, glossy and apparently stable but microscopic examination showed J221M version to be a much better emulsion. The density of the internal phase droplets is probably responsible for the increased viscosity. It was the most liked of the three versions.



## **Multi Domain Silicone in Emulsions**

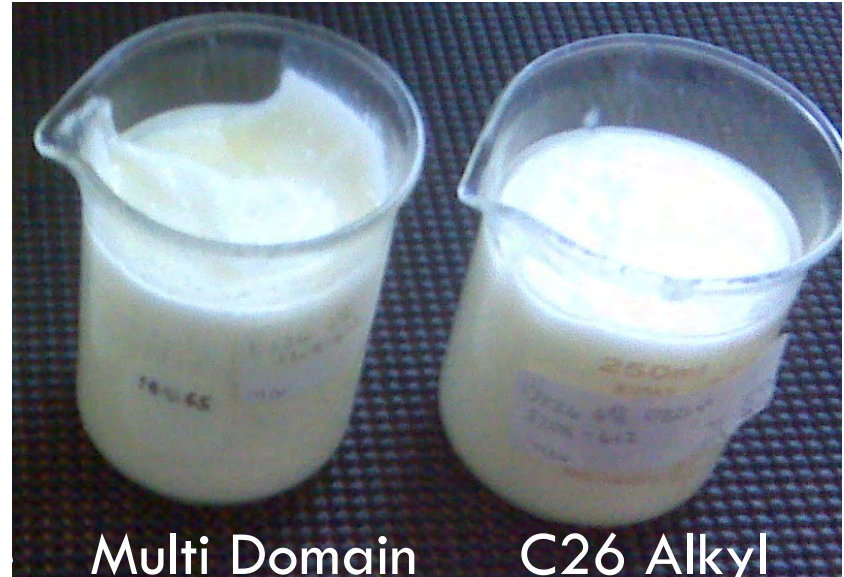




# Structured Emulsion



Cetyl dimethico



Multi Domain

C26 Alkyl

Material	Non-Structured Gel (%)	Structured (%)
Olive Oil	36.0	36.0
Water	56.0	56.0
Silube J208-612	4.0	4.0
Alkyl Silicone	4.0	4.0

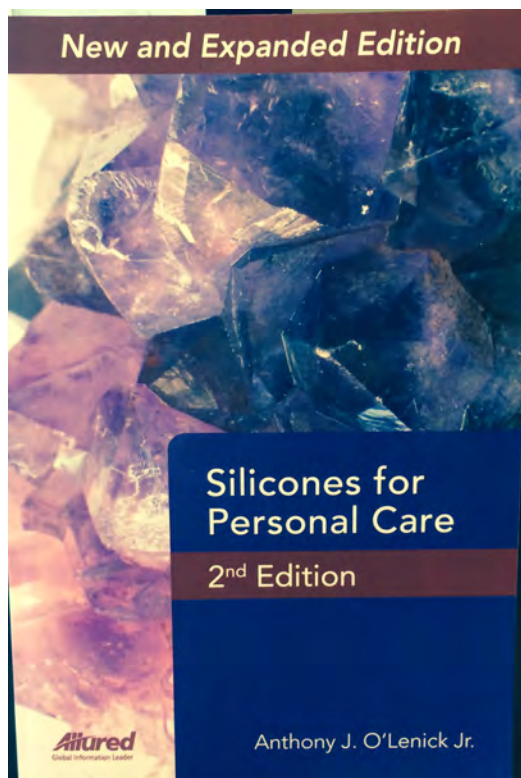


# Alkyl Silicones

1. Can lower surface tension of oils, esters, hydrocarbons and triglycerides, which can alter aesthetics.
2. Can be used to form gels in oils, esters, hydrocarbons and triglycerides, which are free of trans-fats.
3. Can contribute to aesthetics of formulations including serums, creams and lotions.
4. Can be optimized to provide desired effects in formulations



Questions ?





INNOVATIVE SILICONE SPECIALTIES



Thank You

[www.siltechpersonalcare.com](http://www.siltechpersonalcare.com)