



Silwax®



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Alkyl Silicones

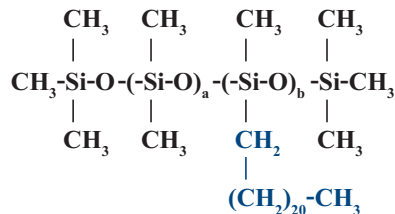
Background

Dimethicone is a very unique material because of its insolubility in both water and oil. This property makes the dimethicone unique, but can also limit its use in formulations. In order to overcome formulation difficulties, dimethicone can be modified to include oil soluble or water-soluble groups. Dimethicone copolyol compounds result in cases where water-soluble groups are added, and alkyl silicones result with the addition of oil soluble groups. It is this latter group that is addressed in this brochure.

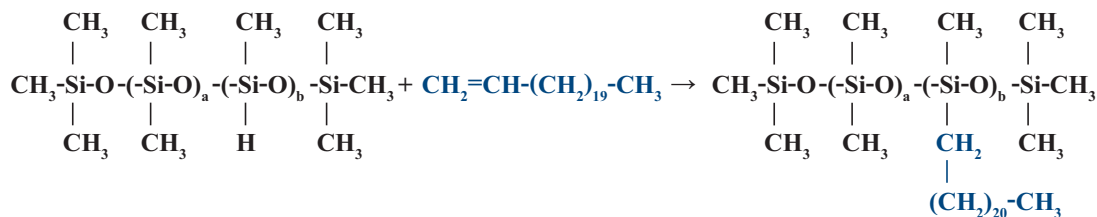
The addition of oil soluble groups to the silicone backbone results in materials that are highly desirable in personal care formulations. Unlike dimethicone, alkyl dimethicone compounds are soluble in oils including mineral oil, esters and other oily phases, due to the presence of the alkyl group. The beneficial properties of silicone are also seen such as lowering of surface tension making the oil feel more like silicone. The presence of two groups, oil soluble and silicone soluble, in the same molecules, these molecules are surface active, going to the interface first then forming micelles. The molecules orientate on the surface of hair and skin.

Alkyl Silicones Chemistry

Alkyl dimethicone polymers are a class of amphiphilic silicones that have both an alkyl and a silicone portion present in the same molecule. Mutually insoluble groups include water, oil, silicone and fluorocarbon.



Alkyl dimethicone compounds are made by the reaction of a silanic hydrogen containing polymer and an alpha olefin.



Silanic Hydrogen Polymer

C22 Alpha Olefin

Behenyl Dimethicone

Physical Properties

Solubility

Alkyl silicones are insoluble in water, isopropanol, and dimethicone. They are soluble in mineral oil, triglycerides and fatty esters. Their solubility in oily materials makes these products of interest in personal care applications.

Despite the fact that alkyl silicones are soluble in many oils, they go to the surface, lowering surface tension then as the concentration increases form micelles. It is this property of alkyl silicones that offer the formulator the most advantage. The lowering of surface tension from 30 dynes/cm² to 20 dynes/cm² makes the oil based product feel more like silicone.

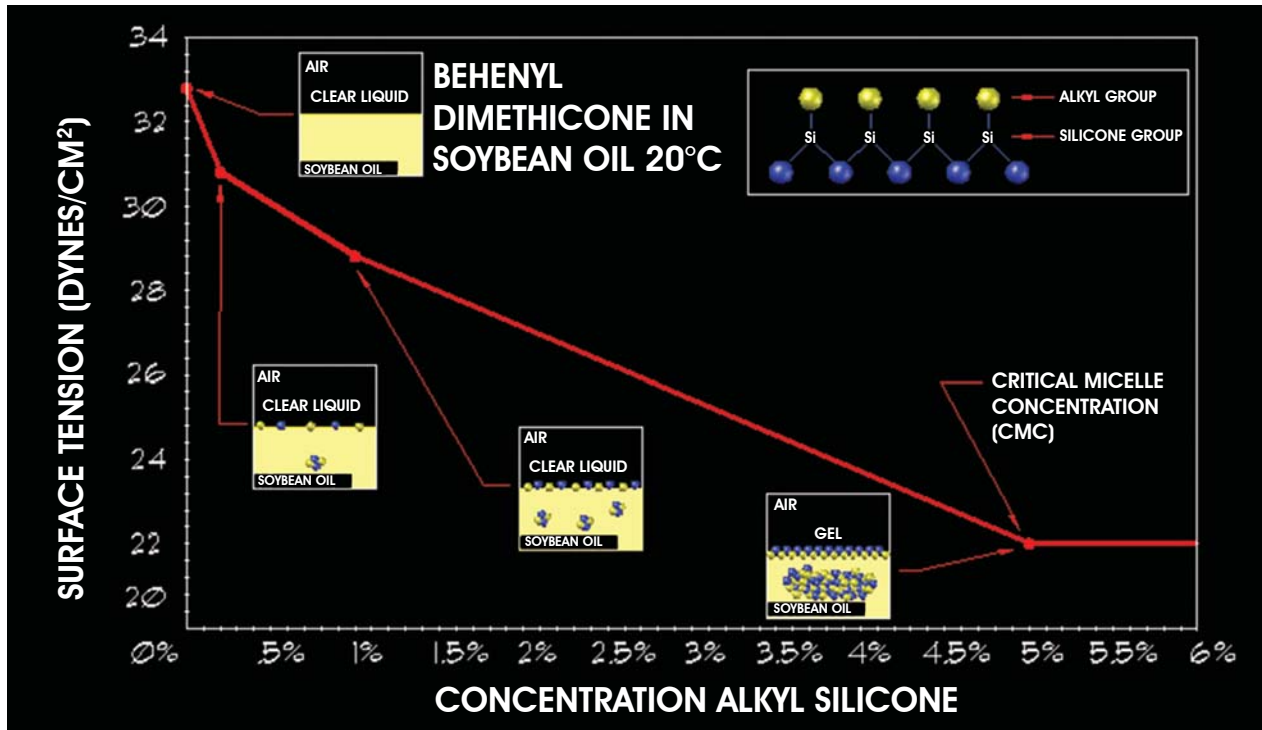
The melt point of an alkyl dimethicone is determined in large part by the length of the alkyl group attached to the silicone. The amount of silicone can also effect the melt point, but to a lesser degree. The amount of silicone present on the molecule alters the hardness of the alkyl dimethicone. As the amount of silicone increases in a molecule, the material becomes softer.

Typical values for alkyl dimethicone products having alkyl chains are: C-22 alkyl 35°C; C-26 alkyl 50°C and C-32 alkyl 60°C.



Surfactant Properties

The graphic below demonstrates that the alkyl dimethicone firstly lowers surface tension by going to the air-oil interface. As the concentration of alkyl silicone increases, micelles form in the oil phase. If the proper alkyl silicone is chosen, a gel is formed. This ability to gel oils results in many cosmetically elegant products.



Surfactant properties in solution

Standard Alkyl Dimethicone Line

Typical Silwax® Products

Alkyl dimethicone compounds are designed for enhanced oil solubility and to change the feel and aesthetics of personal care products. This is achieved by incorporating oil soluble alkyl and/or aryl groups, either in the terminal position on the silicone molecule or at the terminal ends.

- Placement of the alkyl group on the terminal portion of the silicone polymer provides a softer lower melting wax than if the same alkyl group is placed in a comb structure.
- The higher the number of carbon atoms in the alkyl group, the higher the melt point and the harder the wax.
- Aromatic groups placed on the silicone increase refractive index and gloss.
- Lower viscosity products spread better in oil phase giving the oil a more silicone like feel.

This ability to alter the ratio of alkyl groups to silicone group and the ability to choose the length of the alkyl group allows us to customize this class of compounds for specific applications. A specific hardness can be achieved within a specified melt point. This has profound implications on formulations.

Standard Alkyl Dimethicone Line (Continued)

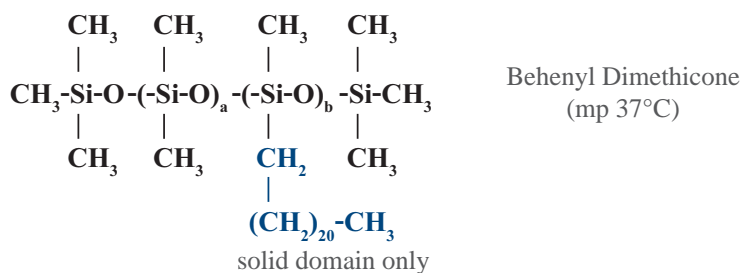
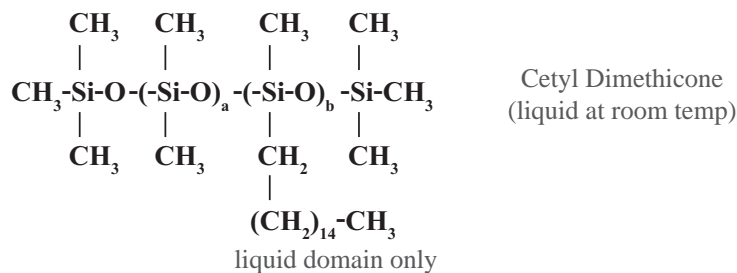
Product	INCI Name	Appearance	Melt Point	Comments
Silwax B116	Cetyl Dimethicone	Liquid	Liquid	Low viscosity, C16 alkyl
Silwax H416	Cetyl Dimethicone	Liquid	Liquid	Mid viscosity, C16 alkyl
Silwax 3H-MS	Isopropyl Phenyl Dimethicone	Liquid	Liquid	Aromatic high gloss
Silwax D0-MS	Isopropyl Phenyl Dimethicone	Liquid	Liquid	Aromatic high gloss
Silwax Di-5026	Ceretyl Dimethicone	Solid	30°C	C26 terminal alkyl
Silwax D222	Behenyl Dimethicone	Solid	37°C	C22 alkyl
Silwax D226	Ceretyl Dimethicone	Solid	47°C	C26 alkyl
Silwax J1032	C-32 Alkyl Dimethicone	Solid	60°C	C32 alkyl



States of Matter

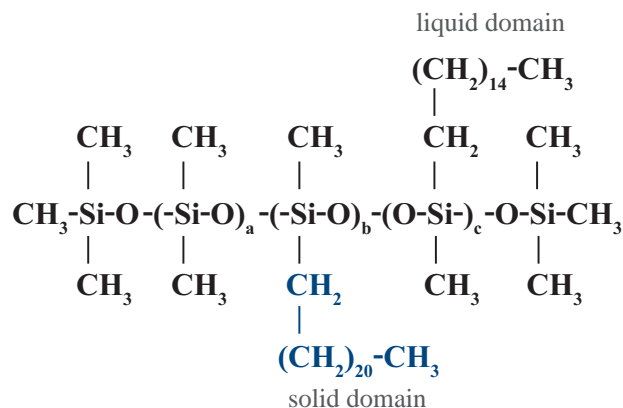
A solid is a state of matter in which the material shows resistance to deformation and changes in volume. Solids have their molecules closely packed together in fixed positions. If the molecules are fixed in repeating groups a crystalline group occurs. A liquid is a state of matter in which molecules are fluid that is they can move easily around, assuming the shape of the container.

Alkyl dimethicone compounds have been around for many years. They are soluble in a variety of oils like mineral oil, and esters. The length of the alkyl chain determines the melt point of the traditional alkyl dimethicone. Consequently, cetyl (C16) dimethicone is liquid and Behenyl dimethicone (C22) is solid.



Multi Domain Silicones

Unlike the products shown above, Multi-domain silicone polymers are carefully engineered materials that have segments called domains that have both solid and liquid alkyl groups placed on the same silicone backbone. The result is an inability to form a hard wax. The reason for this is that the molecule takes on the lowest energy confirmation in which there are solid domains and liquid domains within the matrix. The presence of these different domains within the polymer results in unique properties. The liquid and solid domains within the same molecule limit the ability to form hard solids and result in soft cosmetically elegant wax.



Comparison

A comparison of the multi-domain silicone polymer and product made by blending two silicone polymers on which there is one alkyl group each is shown below. The two products have the same average composition, but the multi-domain product is clearly different. This difference is because of the structuring provided by the multi domain design.

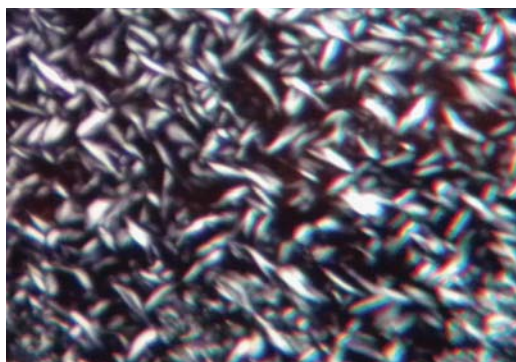
Comparison

Multi-Domain alkyl silicone and blend of two different alkyl silicone polymers (having the same ratio of alkyl groups)

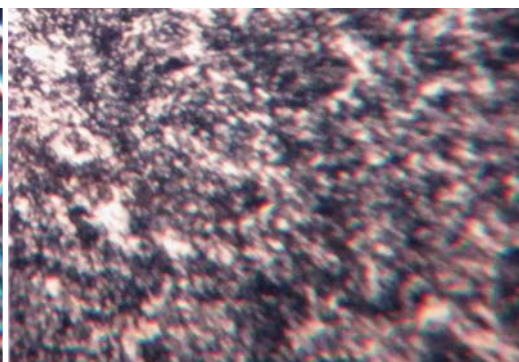


Multi domain alkyl silicone

Blend of two alkyl silicones



Multi Domain Wax
Highly structured crystals
having liquid domains



Blend Alkyl Wax
Standard wax structure

The comparison above clearly demonstrates that the effect of a multi domain alkyl silicone polymer. The product on the left is translucent, and flows slightly. The blended product is hard and opaque. The Multi domain silicone is thixotropic liquefying under pressure feels like petrolatum on the skin but has minimal playtime. It spreads rapidly and has no stickiness. This is attributed to the low surface tension and spreadability provided by the two domains in the one molecule.



Multi Domain Silicone™ Product Line

There are currently four materials in the patent pending Multi Domain Silicone™ product line. The main differences include melt point and skin feel. The products have been described as transient petrolatum, providing the feel and cushion of petrolatum, but has variable playtime, ranging from very little play time to longer play time. Products leave a high level of gloss and no tack, for this reason they have been called “Vanishing Petrolatum”. When added to emulsions, both invert and regular, the effect is dramatic, providing outstanding skin feel. When added to shampoos as a conditioning agent in coacervate applications, they are oily soluble conditioning agents with outstanding spreadability and dry conditioning. When added to pigmented products, these materials minimize syneresis and improve glide.

Typical Properties

The products do not differ in their solubility activity or appearance.

Appearance	White Gel
Active Content %	100
Color, Gardner	3 Max
Solubility (1% and 10%):	
-Water	-Insoluble
-IPA	-Insoluble
-Mineral Oil	-Soluble
-Cyclopentasiloxane (D5)	-Insoluble
-350 visc. Silicone Fluid	-Insoluble



Product	Melt Point Range (°C)	Carbon Number	Play Time 1 is least 4 is most	Cushion 1 is least 4 is most	Description
Silwax D221M	34-36	21	2	1	Comb Silicone
Silwax J221M	30-33	21	3	2	Higher MW Silicone than D-221M
Silwax J218M	29-32	18	4	4	Higher MW Silicone and lower carbon number than D-221M
Silwax Di1021M	35-38	21	1	3	Terminal Functionality

Uses and Applications

The **MULTI DOMAIN SILICONE SILWAX®** product line provide gloss, softness, barrier properties and lubrication. The salient differences is found in melt point, play time, gloss and cushion. These materials are useful in sun care products to increase SPF, moisturizers, lotions, antiperspirants and deodorants and pigmented products (lipsticks, mascara, foundations). Typical formulations available upon request.



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