

Polydimethylsiloxane

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Polydimethylsiloxane (PDMS) belongs to a group of polymeric organosilicon compounds that are commonly referred to as silicones.^[1] PDMS is the most widely used silicon-based organic polymer, and is particularly known for its unusual rheological (or flow) properties. PDMS is optically clear, and, in general, inert, non-toxic, and non-flammable. It is also called **dimethicone** and is one of several types of silicone oil (polymerized siloxane). Its applications range from contact lenses and medical devices to elastomers; it is also present in shampoos (as dimethicone makes hair shiny and slippery), food (antifoaming agent), caulking, lubricants, kinetic sand , and heat-resistant tiles.

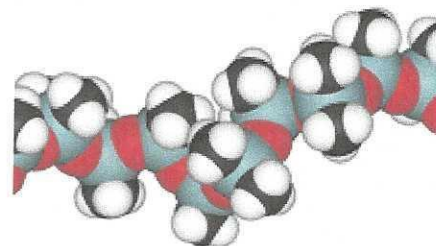
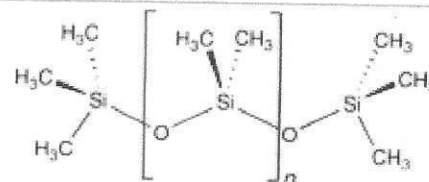
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Structure

The chemical formula for PDMS is $\text{CH}_3[\text{Si}(\text{CH}_3)_2\text{O}]_n\text{Si}(\text{CH}_3)_3$, where n is the number of repeating monomer $[\text{SiO}(\text{CH}_3)_2]$ units.^[2] Industrial

Polydimethylsiloxane



Names

IUPAC name

poly(dimethylsiloxane)

Other names

PDMS

dimethicone

dimethylpolysiloxane

E900

Identifiers

CAS Registry Number

63148-62-9 ✓

ATC code

P03AX05

ChemSpider

✓

UNII

92RU3N3Y1O ✓

Properties

Chemical formula

$(\text{C}_2\text{H}_6\text{OSi})_n$

Density

965 kg m^{−3}

Melting point

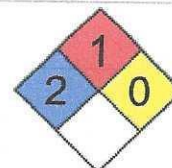
N/A (vitrifies)

Boiling point

N/A (vitrifies)

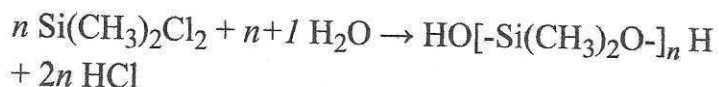
Hazards

NFPA 704



Except where otherwise noted, data are given for

synthesis can begin from dimethyldichlorosilane and water by the following net reaction:



materials in their standard state (at 25 °C [77 °F], 100 kPa).

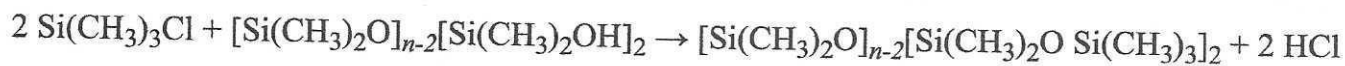
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Infobox references

The polymerization reaction evolves hydrogen chloride. For medical and domestic applications, a process was developed in which the chlorine atoms in the silane precursor were replaced with acetate groups. In this case, the polymerization produces acetic acid, which is less chemically aggressive than HCl. As a side-effect, the curing process is also much slower in this case. The acetate is used in consumer applications, such as silicone caulk and adhesives.

Branching and capping

Hydrolysis of $\text{Si(CH}_3)_2\text{Cl}_2$ generates a polymer that is terminated with silanol groups ($-\text{Si(CH}_3)_2\text{OH}$). These reactive centers are typically "capped" by reaction with trimethylsilyl chloride:



Silane precursors with more acid-forming groups and fewer methyl groups, such as methyltrichlorosilane, can be used to introduce branches or cross-links in the polymer chain. Under ideal conditions, each molecule of such a compound becomes a branch point. This can be used to produce hard silicone resins. In a similar manner, precursors with three methyl groups can be used to limit molecular weight, since each such molecule has only one reactive site and so forms the end of a siloxane chain.

Well-defined PDMS with a low polydispersity index and high homogeneity is produced by controlled anionic ring-opening polymerization of hexamethylcyclotrisiloxane. Using this methodology it is possible to synthesize linear block copolymers, heteroarm star-shaped block copolymers and many other macromolecular architectures.

The polymer is manufactured in multiple viscosities, ranging from a thin pourable liquid (when n is very low), to a thick rubbery semi-solid (when n is very high). PDMS molecules have quite flexible polymer backbones (or chains) due to their siloxane linkages, which are analogous to the ether linkages used to impart rubberiness to polyurethanes. Such flexible chains become loosely entangled when molecular weight is high, which results in PDMS' unusually high level of viscoelasticity.

Mechanical properties

PDMS is viscoelastic, meaning that at long flow times (or high temperatures), it acts like a viscous liquid, similar to honey. However, at short flow times (or low temperatures), it acts like an elastic solid, similar to rubber. In other words, if some PDMS is left on a surface overnight (long flow time), it will flow to cover the surface and mold to any surface imperfections. However, if the same PDMS is rolled into a sphere and thrown onto the same surface (short flow time), it will bounce like a rubber ball.^[2]

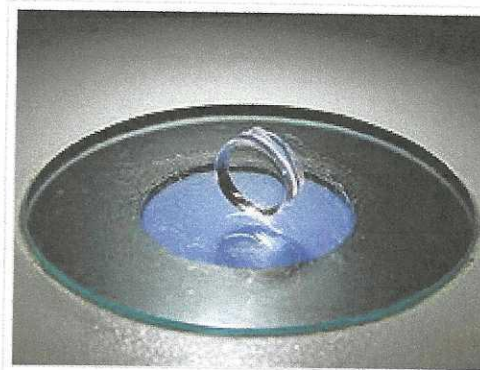
Although the viscoelastic properties of PDMS can be intuitively observed using the simple experiment described above, they can be more accurately measured using dynamic mechanical analysis. This method requires determination of the material's flow characteristics over a wide range of temperatures, flow rates,

and deformations. Because of PDMS's chemical stability, it is often used as a calibration fluid for this type of experiment.

The shear modulus of PDMS varies with preparation conditions, but is typically in the range of 100 kPa to 3 MPa. The loss tangent is very low ($\tan \delta \ll 0.001$).^[3]

Chemical compatibility

After polymerization and cross-linking, solid PDMS samples will present an external hydrophobic surface.^[4] This surface will appear metallic and shiny, although the substrate is clear. This surface chemistry makes it difficult for polar solvents (such as water) to wet the PDMS surface, and may lead to adsorption of hydrophobic contaminants. Plasma oxidation can be used to alter the surface chemistry, adding silanol (SiOH) groups to the surface. Atmospheric air plasma & argon plasma will work for this application. This treatment renders the PDMS surface hydrophilic, allowing water to wet it. This is frequently required for water-based microfluidics. The oxidized surface resists adsorption of hydrophobic and negatively charged species. The oxidized surface can be further functionalized by reaction with trichlorosilanes. After a certain amount of time, recovery of the surface's hydrophobicity is inevitable, regardless of whether the surrounding medium is vacuum, air, or water; the oxidized surface is stable in air for about 30 minutes.^[5]



Hardened PDMS cylinder on the glass of a stereomicroscope light.

Solid PDMS samples (whether surface oxidized or not) will not allow aqueous solvents to infiltrate and swell the material. Thus PDMS structures can be used in combination with water and alcohol solvents without material deformation. However most organic solvents will diffuse into the material and cause it to swell,^[4] making them incompatible with PDMS devices. Despite this, some organic solvents lead to sufficiently small swelling that they can be used with PDMS, for instance within the channels of PDMS microfluidic devices. The swelling ratio is roughly inversely related to the solubility parameter of the solvent. Diisopropylamine swells PDMS to the greatest extent; solvents such as chloroform, ether, and THF swell the material to a large extent. Solvents such as acetone, 1-propanol, and pyridine swell the material to a small extent. Alcohols and polar solvents such as methanol, glycerol and water do not swell the material appreciably.^[6]

Applications

Surfactants and antifoaming agents

PDMS is a common surfactant and is a component of defoamers, which are used to suppress the formation of foams.^[7] PDMS in a modified form is used as an herbicidal penetrant^[8] and is a critical ingredient in water-repelling coatings, such as Rain-X.^[9]

Hydraulic fluids and related applications

Dimethicone is also the active silicone fluid in automotive viscous limited slip differentials and couplings. This is usually a non-serviceable OEM component but can be replaced with mixed performance results due to variances in effectiveness caused by refill weights or non-standard pressurizations.

Soft lithography

PDMS is commonly used as a stamp resin in the procedure of soft lithography, making it one of the most common materials used for flow delivery in microfluidics chips.^[10] The process of soft lithography consists of creating an elastic stamp, which enables the transfer of patterns of only a few nanometers in size onto glass, silicon or polymer surfaces. With this type of technique, it is possible to produce devices that can be used in the areas of optic telecommunications or biomedical research. The stamp is produced from the normal techniques of photolithography or electron-beam lithography. The resolution depends on the mask used and can reach 6 nm.^[11]

In biomedical (or biological) microelectromechanical systems (bio-MEMS), soft lithography is used extensively for microfluidics in both organic and inorganic contexts. Silicon wafers are used to design channels, and PDMS is then poured over these wafers and left to harden. When removed, even the smallest of details is left imprinted in the PDMS. With this particular PDMS block, hydrophilic surface modification is conducted using plasma etching techniques. Plasma treatment disrupts surface silicon-oxygen bonds, and a plasma-treated glass slide is usually placed on the activated side of the PDMS (the plasma-treated, now hydrophilic side with imprints). Once activation wears off and bonds begin to reform, silicon-oxygen bonds are formed between the surface atoms of the glass and the surface atoms of the PDMS, and the slide becomes permanently sealed to the PDMS, thus creating a waterproof channel. With these devices, researchers can utilize various surface chemistry techniques for different functions creating unique lab-on-a-chip devices for rapid parallel testing.^[12] PDMS can be cross-linked into networks and is a commonly used system for studying the elasticity of polymer networks. PDMS can be directly patterned by surface-charge lithography.^[13]

PDMS is being used in the making of synthetic Gecko adhesion dry adhesive materials, to date only in laboratory test quantities.^[14]

Some flexible electronics researchers use PDMS because of its low cost, easy fabrication, flexibility, and optical transparency.^[15]

Medicine and cosmetics

Activated dimethicone, a mixture of polydimethylsiloxanes and silicon dioxide (sometimes called simethicone), is often used in over-the-counter drugs as an antifoaming agent and carminative.^{[16][17]} It has also been at least proposed for use in contact lenses.^[18]

Skin

PDMS is used variously in the cosmetic and consumer product industry as well. For example, PDMS can be used in the treatment of head lice on the scalp^[19] and dimethicone is used widely in skin-moisturizing lotions where it is listed as an active ingredient whose purpose is "skin protection." Some cosmetic

formulations use dimethicone and related siloxane polymers in concentrations of use up to 15%. The Cosmetic Ingredient Review's (CIR) Expert Panel, has concluded that dimethicone and related polymers are "safe as used in cosmetic formulations."^[20]

Hair

PDMS compounds such as amodimethicone, are effective conditioners when formulated to consist of small particles and be soluble in water or alcohol/act as surfactants^{[21][22]} (especially for damaged hair^[23]), and are even more conditioning to the hair than common Dimethicone and/or Dimethicone copolyols.^[24]

Foods

PDMS is added to many cooking oils (as an antifoaming agent) to prevent oil splatter during the cooking process. As a result of this, PDMS can be found in trace quantities in many fast food items such as McDonald's Chicken McNuggets and French fries,^[25] and Wendy's French fries.^[26]

Domestic and niche uses

Many people are indirectly familiar with PDMS because it is an important component in Silly Putty, to which PDMS imparts its characteristic viscoelastic properties.^[27] Another toy PDMS is used in is Kinetic Sand. The rubbery, vinegary-smelling silicone caulks, adhesives, and aquarium sealants are also well-known. PDMS is also used as a component in silicone grease and other silicone based lubricants, as well as in defoaming agents, mold release agents, damping fluids, heat transfer fluids, polishes, cosmetics, hair conditioners and other applications. PDMS has also been used as a filler fluid in breast implants.

It can be used as a sorbent for the analysis of headspace (dissolved gas analysis) of food.^[28]

Safety and environmental considerations

According to Ullmann's Encyclopedia, no "marked harmful effects on organisms in the environment" have been noted for siloxanes. PDMS is nonbiodegradable, but is absorbed in waste water treatment facilities. Its degradation is catalyzed by various clays.^[29]

See also

- Silicone
- Cyclomethicone
- Siloxanes and other organosilicon compounds
- Polymethylhydrosiloxane (PMHS)
- Silicone rubber

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