INDUSTRY BROCHURE 323

Use of Fumed Silica in **Optically Clear SMP Formulations**

Leading Beyond Chemistry

Use of Fumed Silica in Optically Clear SMP Formulations

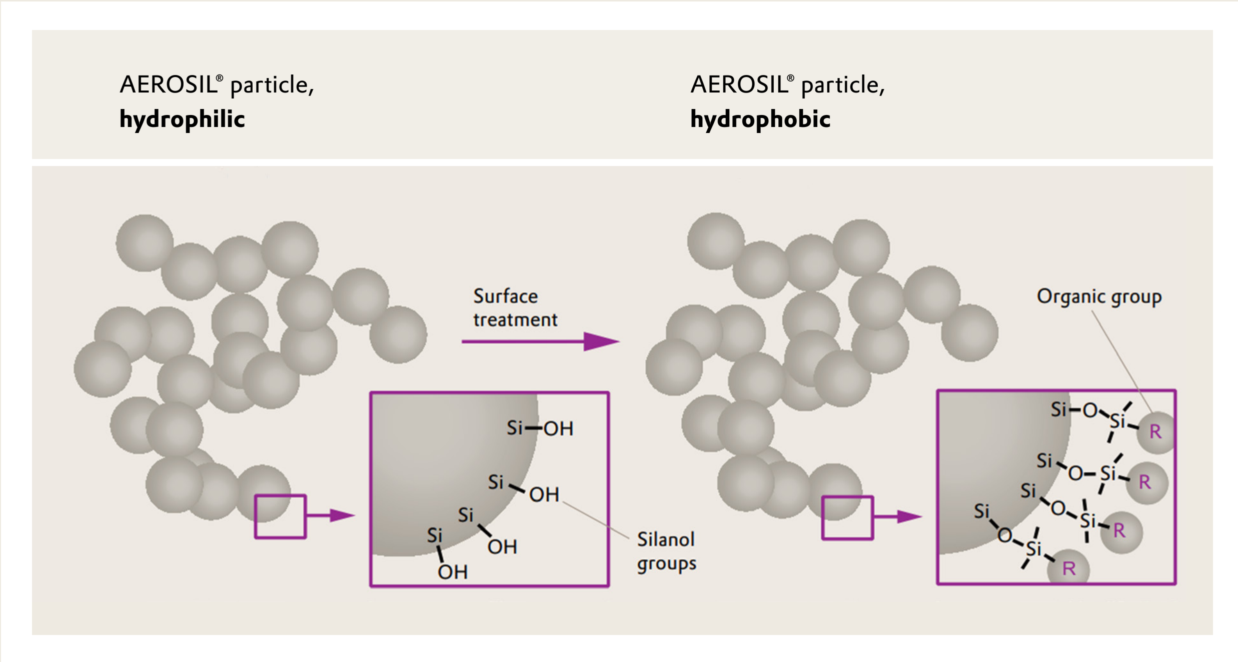
Silane-Modified Polymers (SMPs) are a class of polymer characterized by an organic polymer backbone terminated with organofunctional silane groups, and may also contain urethane groups linking the silane and polymer backbone.

SMPs are further subdivided into two categories: Silyl-Modified Polyurethanes (SPURs) which are comprised of a polyurethane backbone, and Silyl-Modified Polyethers (MS Polymers), comprised of a polyether backbone. The ease of use of these materials (atmospheric moisture curing of one-component products), coupled with their inherent EHS benefits (isocyanate- and solvent-free) and properties that are considered a "hybrid" between traditional silicone and polyurethane technologies, have led to their increased utilization in adhesive and sealant applications.

Despite the beneficial properties of these polymer systems, additional reinforcement and rheological modification are typically required. Hydrophobic silicas are the most appropriate products for these purposes in silane-modified polymer systems. Hydrogen bonding potential of the silica is reduced by reacting hydrophobizing agents to the silica's surface silanol groups.
This results in:

- Lower moisture absorption capacity vs. hydrophilic grades
- Lower levels of silica agglomeration that yields better dispersion
- Greater SMP shelf-life stability (via the reduction in moisture absorption)
- Efficient rheological modification in more polar resin systems, such as SMPs

Figure 1

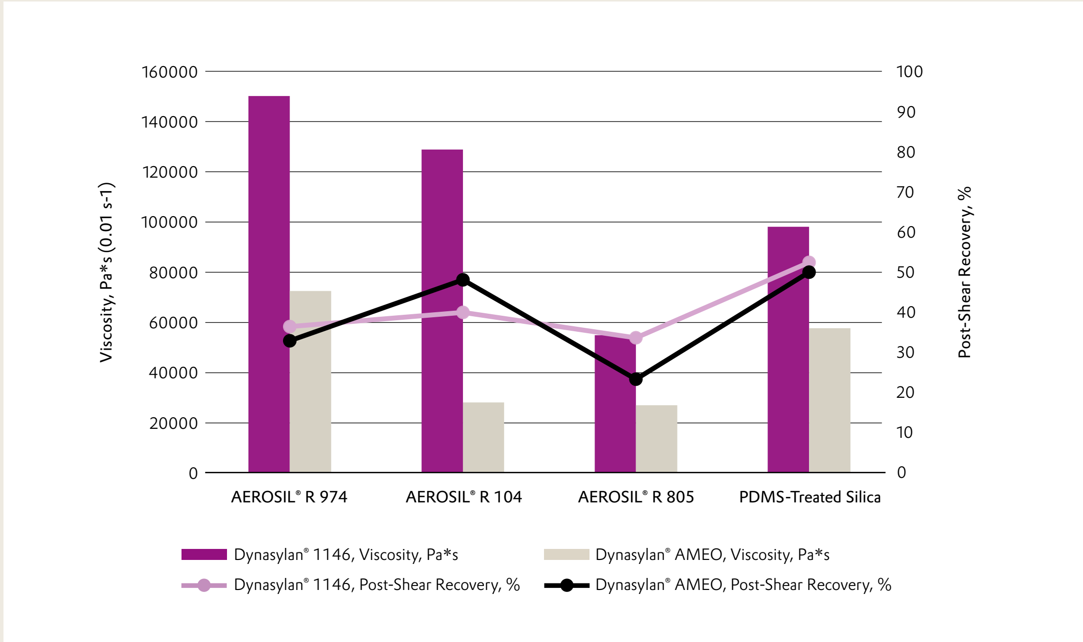


Influence of Silica and Silane Combinations on Rheological Behavior

Functional silanes are widely used in SMP systems as cross-linkers, drying agents, and adhesion promoters. Additionally, functional silanes are known to be capable of hydrolysis reactions with silica surface silanols, as evidenced by some functional silanes being utilized in the hydrophobization process. When silica and silanes are used in combination in SMP systems, there is a pronounced effect on rheological properties. **Figure 2** shows the effect of these interactions between fumed silica and functional silanes, specifically Dynasylan® 1146, on viscosity generation in SMP systems.

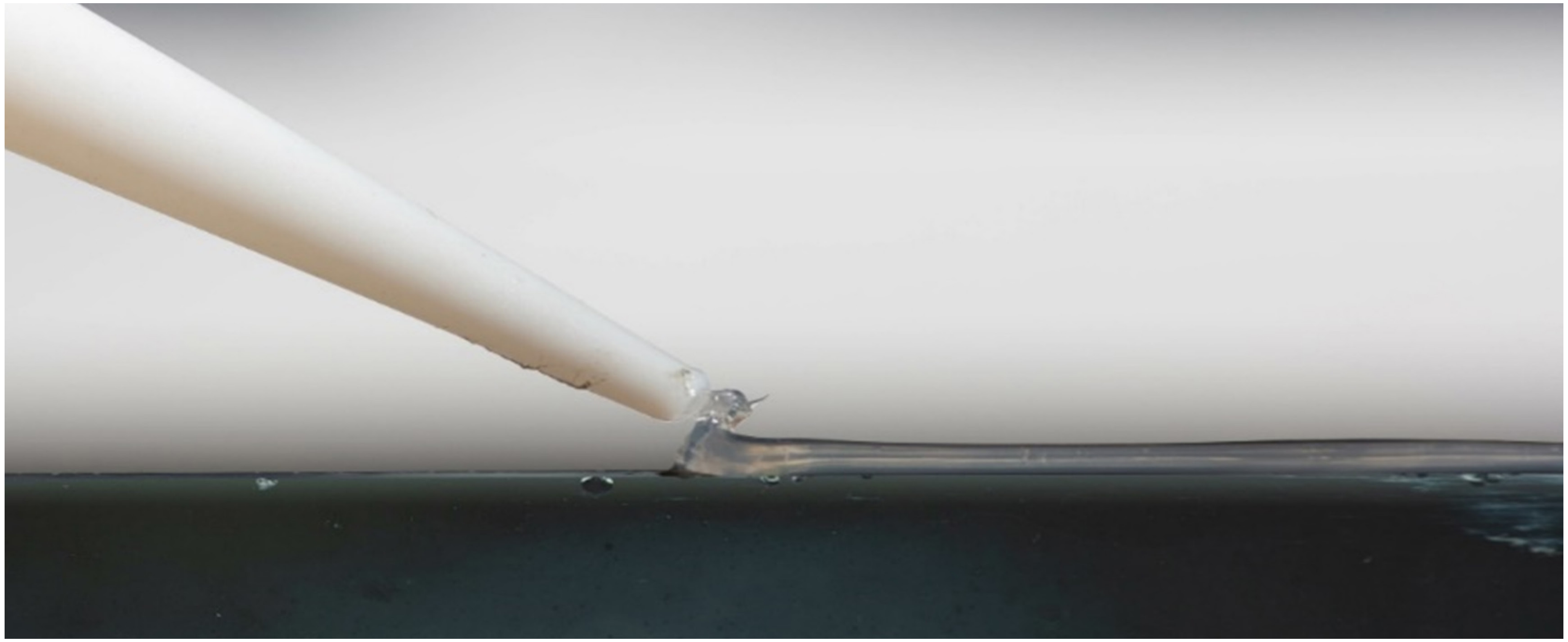
The methoxy-functional oligomer Dynasylan® 1146 and ethoxy-functional Dynasylan® AMEO were utilized in combination with hydrophobic fumed silicas. These observations show the clear benefits of oligomeric methoxy-functional silanes in SMP systems. A more efficient rheological profile is realized when using Dynasylan® 1146 vs. the non-oligomeric ethoxy-functional silane Dynasylan® AMEO. The oligomeric structure of Dynasylan® 1146 contains both amino and alkyl functional groups. Both the length and dual functional groups of the oligomer allow for greater interactions with the fumed silica surface silanol groups, which promotes an improvement in rheological behavior in these systems. This effect is more pronounced with fumed silicas with a lower degree of hydrophobicity and more available surface silanols, which is why AEROSIL® R 974 and AEROSIL® R 104 have higher viscosity values than the more hydrophobic AEROSIL® R 805 and PDMS-treated silica. Regardless of fumed silica selection, Dynasylan® 1146 is the preferred silane to use for rheological behavior in clear SMP systems.

Figure 2



*Silica Concentration: 15 % by weight

Adhesion Performance: Influence of Other Formulation Components on Silica and Silane Combination Performance



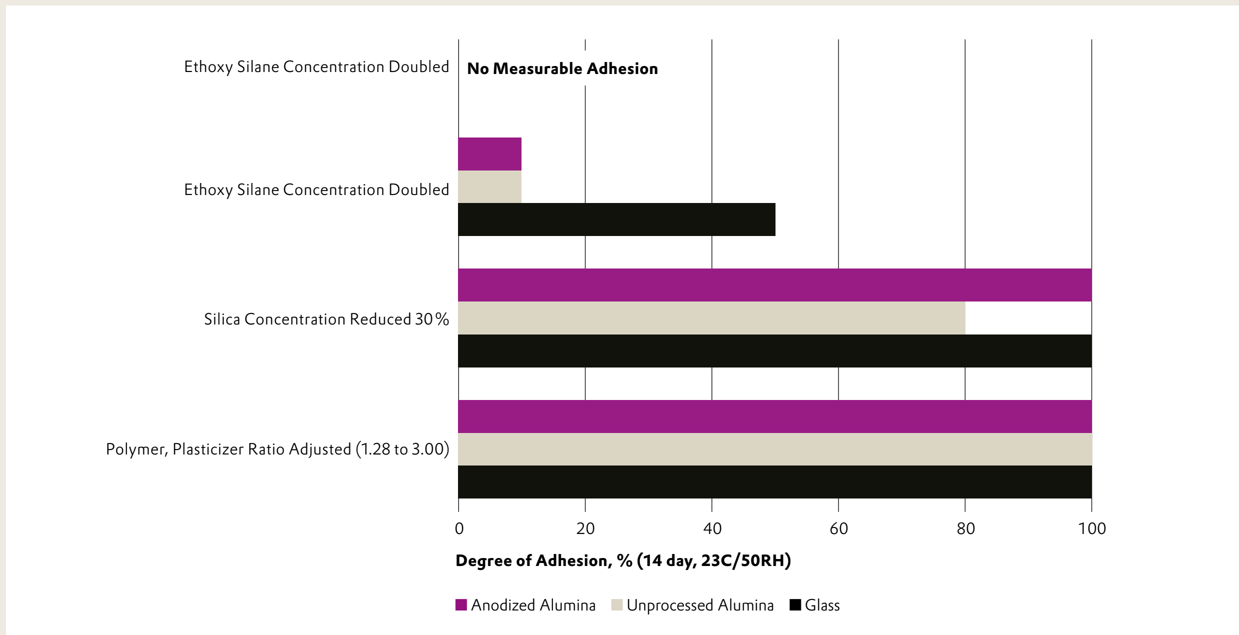
The greatest benefits to adhesion were seen by adjusting several formulation components, both including and excluding silica and silane. Increasing the silane and decreasing the fumed silica concentrations show considerable adhesion benefits. This is likely due to a higher concentration of silane available to form adhesive bonds with the substrate, both by increasing overall silane concentration in the system and a reduced silica concentration yielding fewer in-situ interactions, respectively.

By keeping silica/silane concentrations the same, and adjusting the ratio of polymer to plasticizer more in favor of the polymer, the formulation achieved full adhesion to all three substrates. This indicates that fumed silica and silane performance in SMP adhesives are further improved by additional optimization of the entire formulation, rather than the adhesion profile being entirely driven by the combination of fumed silica and functional silanes.

Unlike the combined effect of silica/silane on rheological performance, where the specific relationship between silane and silica is identified, the effect on adhesion performance is not as clear. It is only clear that silica/silane interactions do have a quantifiable effect on adhesion generation of SMP systems, but the exact correlation between silica/silane interactions and adhesion performance is not currently well understood. It is, however, understood that adhesion performance is multi-factorial, and each silica/silane combination can be improved with further formula optimization.

Figure 3 shows the effect that several formulation components, not limited to silica and silanes, have on adhesion. Beginning with a PDMS-treated silica (AEROSIL® R 202) and ethoxy-functional silane (Dynasylan® AMEO) formula, several formulation adjustments show notable improvements in adhesion. Adhesion testing was performed qualitatively 14 days after the application of material to the substrates, with degree of adhesion corresponding to the amount of cohesive failure of the material. Cohesive failure is evident when the SMP material tears during testing, leaving a thin layer of material still bound to the substrate surface.

Figure 3



*Silica Concentration: 15% by weight

Hydrophobic Fumed Silicas AEROSIL® R 104 and AEROSIL® R 812 S

AEROSIL® R 104 hydrophobic fumed silica is after-treated with octamethylcyclotetrasiloxane (D4) and has a specific surface area of approximately 150 m^2/g. **AEROSIL® R 812 S** hydrophobic fumed silica is after-treated with hexamethyldisilazane (HMDS) and has a specific surface area of approximately 220 m^2/g. For both D4 and HMDS treated grades, there is a low residual chloride content, reducing UV-exposure related yellowing in clear formulations. This results in products that are optimal solutions for SMP systems where high optical clarity is a requirement.

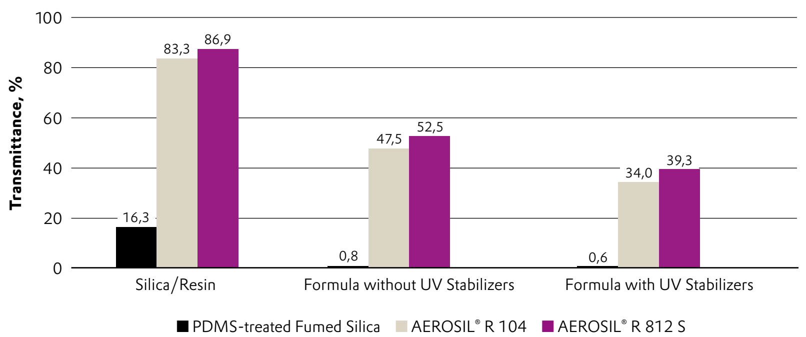
Figure 4

Figure 4 shows resin clarity is well maintained despite a high concentration of hydrophobic fumed silicas AEROSIL® R 812 S and AEROSIL® R 104.

When measuring optical clarity of SMP systems, AEROSIL® R 812 S and AEROSIL® R 104 provide clarity improvements vs. other surface treatment chemistries, such as PDMS in this case. However, other formulation components may have significant impacts on clarity as well.

Figure 5 shows the influence that other traditional formulation components have on optical clarity of the uncured SMP adhesive/sealant when measured by spectrophotometer.

Figure 5



*Silica Concentration: 12 % by weight

Evaluating optical clarity of uncured, clear SMP systems concludes the following:

- AEROSIL® R 812 S and AEROSIL® R 104 maintain high levels of resin optical clarity compared to other fumed silica treatment chemistries
- Additional formulation components (plasticizers, UV stabilizers, etc.) have a greater impact on resin optical clarity compared to AEROSIL® R 104 and AEROSIL® R 812 S

Optically Clear SMP Sealant/Adhesive Guide Formulation

MATERIAL	Wt %
Low-Med Modulus Trimethoxy SMP Polymer, Plasticized with DINCH	55.0
Di-isononyl-1,2-cyclohexanoate	24.75
Dynasylan® VTMO	2.0
Hydrophobically-treated Fumed Silica (AEROSIL® R 104, AEROSIL® R 812 S)	**12.0**
Triazine-based UV Absorber	1.25
Hindered Amine Light Stabilizer	2.0
Aminosilane (Dynasylan® 1146)	**2.0**
Potassium Neodecanoate Catalyst Dilution	1.0

Processing Procedure

- Add full amount of resin, plasticizer, UV additives, and half of the vinyltrimethoxysilane amount and blend these components in mixing vessel
- Add silica (full amount if possible, or divide quantity into vessel with low shear mixing step in between charges), and wet all free flowing silica into the resin blend using low shear conditions
- Increase mixing speed/energy to fully disperse silica in the resin pre-dispersion
- Sequentially add the remaining vinyltrimethoxysilane amount, additional silane coupling agents, and organometallic catalyst; mix under low shear conditions between each addition
- Deaerate material by mixing under low shear conditions at -25 inHg vacuum

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