EFFECT OF SILANE DENSITY ON WETTABILITY OF SILANE-GRAFTED SILICA

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Introduction

- Fiber-matrix adhesion is **critical** for transferring loads effectively and enhancing the overall strength and durability of composites.
  - However, much is still left to be desired when understanding the nanoscale
- Wettability is a governing factor, as emulsion favorability in covering an entire surface directly affects interfacial bond strength and therefore adhesion

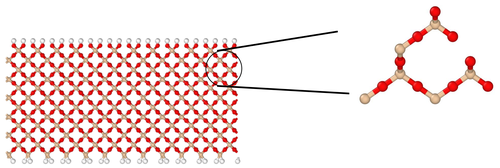


Fig. 1: Molecular Dynamics Model of 10 nm Hydroxylated Q3 Silica

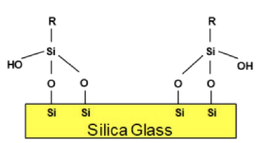


Fig. 2a: Silane agent bonding to S-glass fiber.

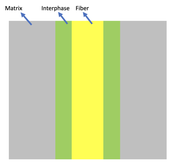


Fig. 2b. Interphase region

- S-glass fibers are commonly used as reinforcement in composite materials, and their surface properties play a crucial role in determining the mechanical behavior of composites
- Our final goal is to understand how multiple Silane chemistry (Glycidoxypropyltrimethoxy (GPS), Aminopropyltriethoxy (APS), and ML derived Silanes) will affect wettability and thereby adhesion

Why?

It is **experimentally challenging** to control the variables which govern the aspects of wettability such as **Bond density,** which is why MD is being utilized

Objectives

- **Realize the effect of Silane-grafted Silica upon the wetting mechanics of a Water Droplet**
  - ✓ Produce literature-backed Silica, Silane, Nitrogen, and Water models
  - ✓ Validate models through extensive testing
  - ✓ Conduct post-analysis of Wetting/Contact angle of Silica

Simulation Details

- Our silica slab utilized the 12-6 OPLSAA Force Field derived parameters from literature

$$V(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

- We investigated the SPC, TIP3P, and TIP4P water model

Model:	SPC	TIP3P	TIP4P
Accurate RDF Plot	✓	✓	✗
Shape Retention at STP	✗	✓	✓

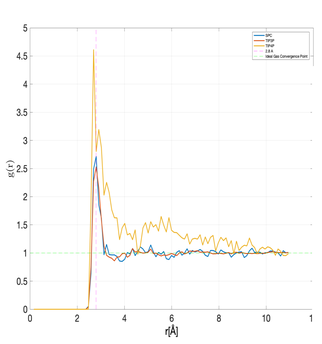


Fig 3a. RDF Plots: TIP3P: Red, SPC: Blue, TIP4P: Yellow

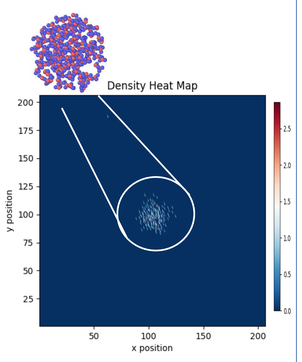


Fig 3b. TIP3P 2.5 nm radius droplet

Results & Discussion

- Our Silica slab consists of an H-bond density of ~7.99 nm^{-2}
- Wettability analysis of Wetting Angle of Hydroxylated Silica

2.5 & 5 nm Diameter Emulsion

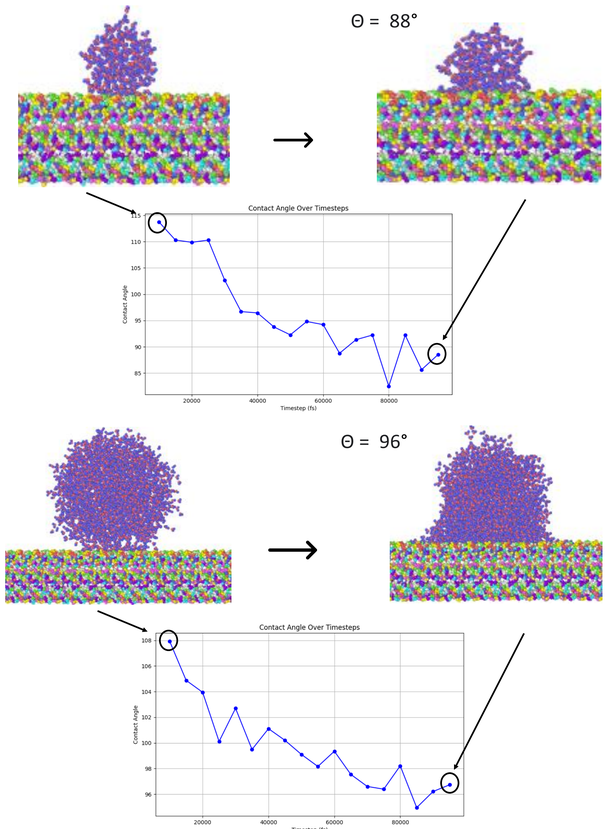


Fig 4. Case studies of 2.5 and 5 nm diameter respectively

- The cases shown above represent a subset of our work, with a contact angle analysis over 100,000 fs. We observe the slow decline and then variation in a quasi-equilibrium state.
- We seek to validate our models through previous literature. A previous study had concerned a Q3 slab, derived from alpha-cristobalite silica.
- As we move forward, we will both conduct experimental studies at the CCM and find more references to which our model can be validation

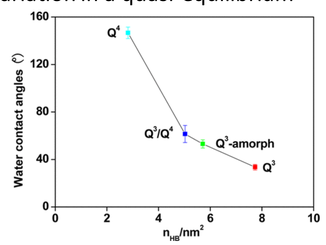
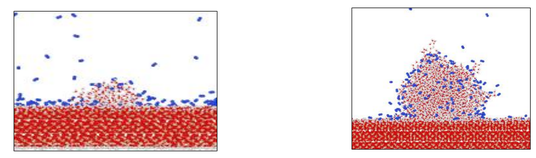


Fig 5. Q3-Q4 Silica slab references

Nitrogen Environment

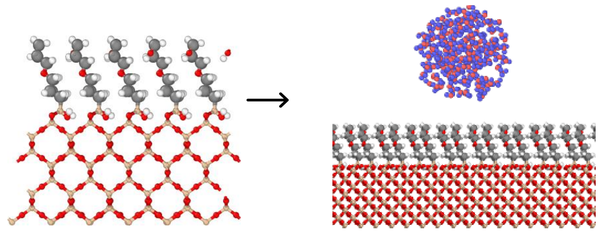
2.5 nm **5 nm**



- We are establishing a scripted-methodology for calculation of the Contact Angle in the Nitrogen Environment

Future Work

- After careful validation of the Silica, Nitrogen, and Water models, we aim to move forward by developing more accurate models to validate the Silica-wetting angle, then more forward to Silane
- We will Validate Silane chemistries such as GPS and APS. Along with this, a ML model will derive new Silanes.



- GPS-grafted Silica is shown above, with a water droplet above representing the next step of our simulations

Acknowledgements

Please include acknowledgements for the support of your work here.

Examples:

This work is supported by the Army Research Laboratory through the Composite Materials Research program.