Simulations of Glass Surfaces: Developing an Understanding of Silane Binding

Modules Used

Materials Studio:
Amorphous Cell, Discover

Industrial Applications

Coatings, Glass

Organizations

Corning. Inc.
Accelrys

Glass slides, coated with γ-aminopropyl triethoxysilane molecules (GAPS – see Fig. 1) have found novel applications such as immobilizing DNA to create microarrays which are widely used in molecular biology. The GAPS molecules are believed to bond covalently to the glass surface via the silane group while leaving a positively charged primary amine group free to attract negatively charged biomolecules such as the phosphate backbone of cDNA. Alternatively, the amine group could be replaced with a nonpolar group and be used to bind non-polar systems such as hydrocarbons to the glass. It is known from experimental studies that the quality of the coating varies depending on the type glass used as substrate.

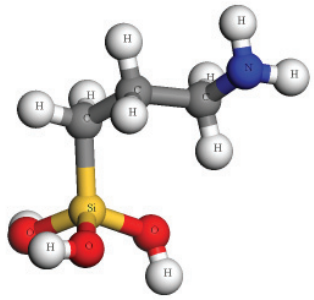

Figure 1 – A molecule of GAPS.

In order to rationalize these observations, scientists at Corning and Accelrys, reporting in the journal Molecular Simulation,[1] used molecular modeling to study the surface of two commonly used glasses; based on sodium silicate and another based on alkaline earth based aluminoborosilicate (AEBS).

Using the Amorphous Cell module, several bulk glasses were constructed and then subject to a quenched annealing approach using the Discover MD code. These methods allow the ions in the glass to gradually come to meta-stable positions similar to those found experimentally. Glass surfaces where created from these bulk structures and annealed using a similar process. This process was repeated 10 times to develop an average of the surface structures possible. The resulting structures were analyzed using several techniques to allow us to compare the differences between the different glasses.

The results show that the sodium silicate glass forms a network of silcon and oxygen atoms, within this matrix clusters of sodium ions are formed which are surrounded by single coordinated non-bridging oxygen atoms. The AEBS glass forms a more complicated networked structure, with boron, aluminum, silicon and oxygen making up the network with the alkaline earth ions uniformly distributed throughout the matrix. This phenomena is seen for the surfaces as well as the bulk (Figs. 2 and 3). Diffusion studies and concentration profiles show that over time the sodium ions in the sodium silicate glass will migrate to the surface. The surface of the AEBS glass shows little segregation of ions and its composition does not change over time. In addition, the AEBS glass surface shows a flatter less corrugated surface.

Consequently, the improved performance of silane coatings on the AEBS glass can be rationalized in terms of :

i) Uniform surface structure and composition of the glass substrate
ii) No change in the substrate composition over time due to segregation of ions to the surface.

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The silane layer formed is more uniform on the glass surface and more importantly the molecules stay bound as there is no change in the surface composition. Thus when selecting suitable substrates to create gene-chips the surfaces must have a uniform composition and show little variation in chemistry over time.

Dr Jim Dickinson, Corning, said, "The computations and experiments proceeded more or less 'hand-in-hand'. If a set of experiments was conducted which showed good binding to one substrate but not the other, it was not always clear from the experimental data why this was so."

"Obviously, hypotheses based on some variation of surface composition, texture, binding sites, and strength could be put forth to explain the results. The computational tools allowed/predicted judgements to be made as to which hypotheses were most valid and pointed to what experiments should be done next. This saved time and money on needless experimentation."

"The scientific advantages of using tools such as these for this type of study are strongly related to understanding how surface composition effects binding. Thus many surface composition changes and their effects can be investigate/predicted and used to guide future experimentation," concluded Dr Dickinson.

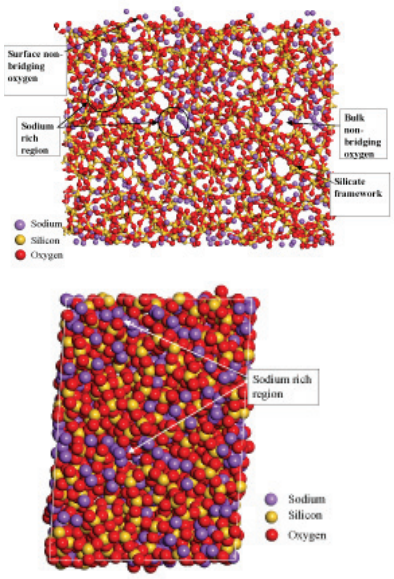

Figure 2 – A view of the sodalime glass surface: (a) parallel to the C-axis and (b) normal to the A and B axis plane

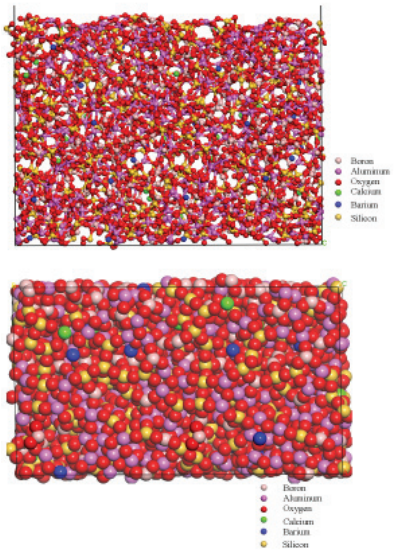

Figure 3 – A view of the AEBS glass surface a) parallel to the C-axis and b) normal to the A and B axis plane

Reference

1. S. Vyas, J. E. Dickinson, and E. Armstrong-Poston, Towards an Understanding of the Behavior of Silanes on Glass: an Atomistic Simulation Study of Glass Surfaces, Molecular Simulation, 2006, 32(2), 135.

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