Tuning Small-Molecule Permeability in Glassy Polymers with Nanoparticles

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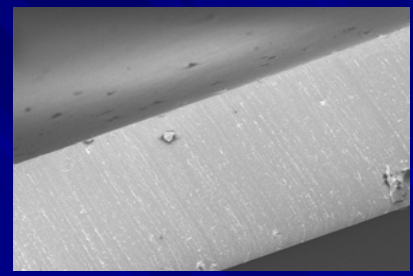
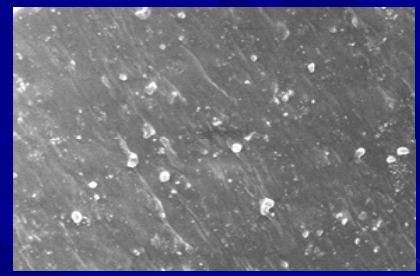
- **Background:** To efficiently and effectively separate gas mixtures, membranes must exhibit both high gas permeability (fast transport) and high selectivity for one gas over the other. Unfortunately, these properties tend to be diametrically opposed: membranes made of rubbery polymers have high permeabilities but low selectivities, while membranes made of glassy polymers have high selectivities but low permeabilities. It has long been accepted that the addition of micron-sized inert impermeable particles to a polymer film decreases the permeability while leaving the selectivity unchanged. However, recent research has shown that adding nanoparticles to a special class of glassy polymers results in an *increase* in permeability, while retaining or possibly even improving the selectivity.

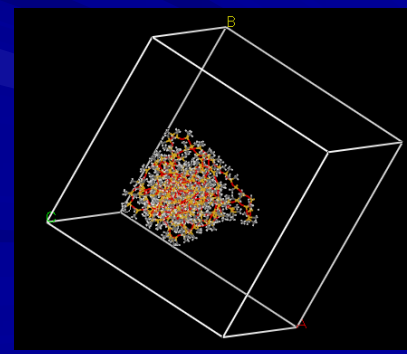
- **Our Work**: We are examining the crossover between permeability enhancement and reduction with changes in particle size and polymer type.
  - **Experimental**: We have developed techniques for casting polymer membranes from poly(dimethyl siloxane) (PDMS), polycarbonate (PC), and poly (ether imide) (PEI). We have also prepared PDMS/silica composite films, and found that the stirring rate affects agglomerate size. We are currently synthesizing silica particles of various sizes using the Stober process, working on surface modification of the particles to reduce agglomeration, and running gas permeation experiments for pure and composite films.
  - **Modeling**: We have begun molecular modeling of the polymers using Accelrys' Materials Studio 4.0. We have developed an equilibration procedure, and are currently setting up a cluster to decrease computational time. We plan to examine the change in free volume upon particle addition and the polymer-particle interface.



SEM micrograph of cross section of PDMS membrane.



SEM micrograph of PDMS composite containing amorphous, untreated silica nanoparticles.



Molecular Dynamics screenshot containing unit cell with a non-equilibrated PDMS chain.