Experimental and theoretical determination of Heliums diffusion coeficient in Kapton®

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Kapton (poly-oxydiphenylene-pyromellitimide) is a polyimide film that is stable throughout a large temperature range of -269 to +400 degrees. This polymer is utilized in a variety of applications, including flexible printed circuits, in spacecraft (aluminized foils to provide thermal insulation), aircraft (for insulated electrical wiring), satellites, as an insulator in ultra-high vacuum environments, as a material for windows used with all kinds of X-ray sources, 3D printing and cryogenics. Since this material is widely employed as an insulator in ultra-high vacuum conditions, it is necessary to investigate gas diffusion/permeation properties. The evaluation of helium diffusion on this material is explored both experimentally and by Molecular Mechanic calculations. The throughput method is used to measure diffusion, permeation and solubility coefficient. The throughput method uses an orifice with known dimensions. Measurements were performed for different temperature in the region from 23 -150 ^{0}C.

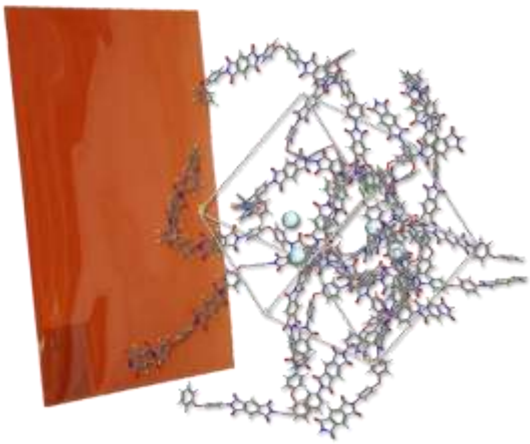

Figure 1. Kapton® film and the PBC model used in theoretical calculations.

Helium's self-diffusion coefficient in Kapton was theoretically determined through the use of Molecular Dynamic simulations. The amorphous cell module was used to build a periodic model consisting of ten chains of poly-oxydiphenylene-pyromellitimide units and five He atoms (Figure 1). This model is geometrically optimized in the first stage (using the COMPASSII forcefield), then exposed to NPT at 0.1MPa (1000 ps), and finally to NVT (3000ps). D=MSD(t)/6 was used to compute the self-diffusion coefficient D (cm^2/s) from the Mean-Square Displacement (MSD) of the helium molecules.