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Description of molecular transport in epoxy-resin and in graphene-epoxy nanocomposite by experimentally determined fractional free volume

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Molecular transport properties of light gases in epoxy-resins membranes with different cross linking density and in epoxy-resins modified with dispersed Few Layer Graphene (FLG) nano-platelets will be discussed in the framework of the free volume theory [1-5].

Four types of resins were prepared by altering their cross-linking densities and hence their glass transition temperature. Nanocomposite membranes were prepared with 1, 5,7.5, 10 wt.% FLG filler content.

PALS measurements were performed with a fast-fast lifetime set-up with a time resolution of 260 ps. The transport of light gases (H_2, N_2, CO_2) was studied by gas phase permeation techniques up to 350 K temperature.

X-ray diffraction, vibrational spectroscopy and scanning electron microscopy analysis were also performed to characterize the structure of the pure and nanocomposite membranes.

Gas phase permeation measurements show that the transport through the pure membranes obeys to the solution diffusion mechanism. Decreasing the cross-linking density both the permeability and the CO_2/N_2 selectivity increases. [1,2]

The fractional free volume $f_h(T)$ and its evolution with the temperature was experimentally evaluated by measuring the hole dimensions by PALS, the thermal expansion coefficient of the hole free volume and the volumetric thermal expansion coefficient.

The gas diffusion constant of CO_2 and the permeability of H_2, N_2 and CO_2 as a function of temperature was reproduced with the free volume theory and using as input parameter the experimentally evaluated fractional free volume $f_h(T)$ data [3,4].

In the nanocomposite membranes dispersion of filler showed a barrier effect on gas transport. PALS analysis indicated that the free volume structure did not change but the fractional free volume decreased with increasing the filler content. Thanks this finding the change of gas transport properties due to fillers was explained and modelled by the formation of a rigidified polymeric region around fillers. [5]

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