Numerical Simulation To Improve The H2O-barrier Property Of Films By Integration Of Water Absorbers

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Abstract

Flexible electronic devices are very sensitive against the ingress of oxygen and water vapor from the atmosphere and therefore must be protected by encapsulation with high barrier films. Typically these films contain at least two or three inorganic barrier layers separated by polymeric layers (lacquer) which are deposited from the liquid or gas phase on top of a flexible substrate. Flexible PV implies new encapsulation challenges coping also with reduction of material quantity, carbon footprint and manufacturing costs. It was found out that the integration of a water vapor absorbing adhesive into the multilayered stack can further enhance the barrier performance. My research focuses mainly on the individual polymeric layers and their barrier performance will be improved as following:
The distinction between the concepts of oxygen- and water vapor barrier structures will be discussed:
a) Polymeric layers with dispersed inorganic particles.
b) Polymeric layers with dispersed permeable water absorbers
Theoretical modelling and numerical simulation of the gas transport processes provide insight into the barrier mechanisms of these structures and make it possible to calculate steady-state and time-dependent permeation rates dependent on geometrical and material parameters. Sorption and diffusion of substances in polymeric layers are described by Henry's and Fick's laws. Since the concentration at the interfaces between two different layers is not a continuous function of place, the partial pressure is used to replace the concentration to describe the water vapor absorption and diffusion through the layers.
The resulting transport equation within the different regions and the conditions at interfaces between the polymeric matrix and the permeable water absorbers govern the transport through one single layer and multilayer structures. The equations were numerically solved by the finite element method using the General Form PDE interface of COMSOL Multiphysics®.
The considered model was applied to the transient permeation through a layer with dispersed permeable water absorbers. Numerical simulations for such a structure show that the period of transient permeation during which the permeation rate approaches the steady-state value is extended due to dispersed permeable, while a relative low increase of the steady-state permeability is observed.

Consequently, the barrier performance of a polymeric layer against water vapor can be significantly improved by its combination with permeable water absorbers. Increasing their volume fraction (size of the particles) and solubility coefficient of permeable particles results in an enhanced effect on the corresponding lag time. Moreover, ensuring a homogeneous dispersion of particles for the layer with water absorbers is not necessary in contrast to the layer with nanoparticles for oxygen barrier.

Figures used in the abstract

Figure 1 : Modelling and simulation for the barrier performance of the layers: partial pressure distribution of the layer with 10 rows of water absorbers

Figure 2 : The streamline plot