BAPVC Annual Project Report

Project Title: Composite encapsulation layers

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Summary:

The group has developed encapsulating layer PV modules using a composite of polymer and water-scavenging nanocrystals. In the first phase, the composite of block copolymer and hygroscopic nanocrystals was used, probing the role of the composite structure and nanocrystals. In this final phase of the project, we build upon both lessons learned from the first phase and feedback from the consortium to move to more scalable systems that can be deployed to partners. Specifically, the group is using more commercially available polymeric system in the second phase with water-scavenging metal organic framework (MOF) molecules.

Key Accomplishments:

The group utilized a self-assembly of block copolymer (poly(styrene-*b*-2-vinylpyridine), PS-P2VP) to modulate the structure of the films. The block copolymer is comprised of hydrophilic (P2VP) and hydrophobic (PS) parts, and its self-assembly results in either spherical (PS-P2VP(S)) or lamellar (PS-P2VP(L)) structure, depending on the ratio of two parts (Figure 1). In both cases, water-scavenging hygroscopic nanocrystals (MgO) are incorporated into hydrophilic blocks. Water vapor molecules are blocked by the hydrophobic layer firstly, and the permeated molecules are absorbed by hydrophilic parts and water-scavenging nanocrystals. Particularly, this water-absorbing process is reversible; hence, the scavenged water molecules can be "breathed-out" again without saturation of the absorbing sites.

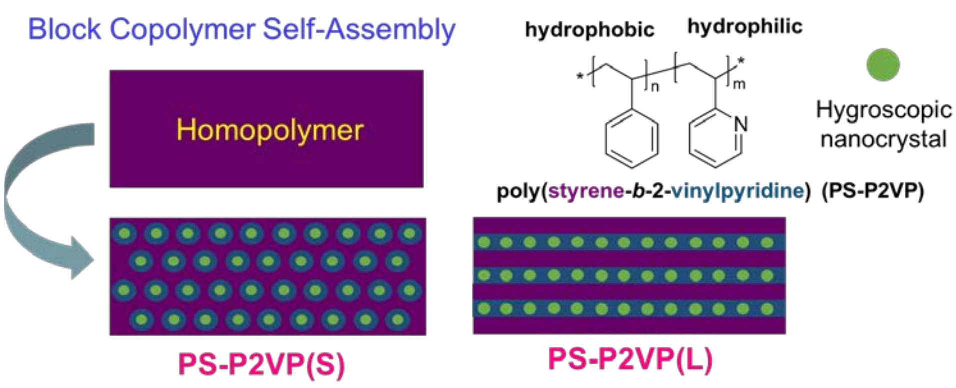

Figure 1. A schematic of the composite films: PS-P2VP(S) and PS-P2VP(L)

Water Vapor Transmission Rate (WVTR) studies showed that our block copolymer system is much more efficient as a barrier layer than the original hydrophobic homopolymer (PS) film, even though the hydrophilic parts are added, which can be attributed to the well-defined internal structure. In addition, the incorporation of hygroscopic nanocrystals (MgO) raised the water-vapor blocking ability of the film to a higher level. Morphologically, it was observed that the sphere structure is more efficient than lamellar.

	WVTR ($g\cdot m^{-2}\cdot day^{-1}$)	WVTR ($g\cdot mil\cdot m^{-2}\cdot day^{-1}$)
PS-P2VP (S)	5.882	$3.076*10^{-3}$
PS-P2VP-MgO (S)	5.719	$2.118*10^{-3}$
PS-P2VP (L)	6.355	$3.285*10^{-3}$
PS-P2VP-MgO (L)	6.184	$2.845*10^{-3}$
PS		7.286

Figure 2. WVTR studies of the composite films

In the first phase, the group learned that the composite of a spherical structure led to more efficient water vapor-blocking; hence, in the second phase they moved to more commercially available base materials as multi-lamellar structures do not offer a clear benefit but only increase cost. The new encapsulating barrier is a composite comprised of hydrophobic COC polymer (cyclic olefin copolymer) and water scavenging MOF nanocrystal to improve the environmental stability and processability, and also functionality and price. The basic idea is an extension of the previous work comprised of PS-P2VP block copolymer and MgO nanoparticle, in which hygroscopic inorganic nanoparticle were incorporated into the copolymer. Already we have fabricated some initial composites for testing at large scale using doctor-blading, and obtained transparent films. Moisture and adhesion tests are underway.

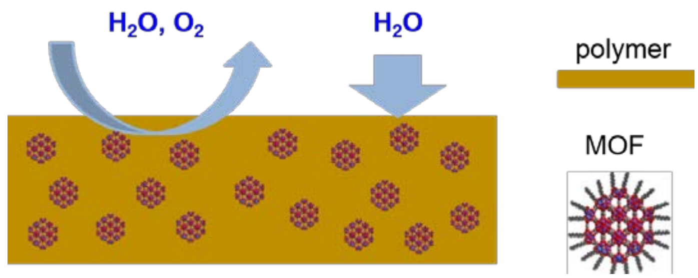

Figure 3. Schematic of the novel composite barrier layer material to under development

Future Work:

The key barrier in this system is to disperse MOF nanocrystal in the polymer matrix, and the group has been working to enhance the dispersibiliy of MOF in hydrophobic solvent. The composite film of COC polymer and MOF with different crystal size will be fabricated using doctor blading, and WVTR value will be measured. Furthermore, the group will test the protection ability of the COC/MOF films by coating the encapsulating materials on different photovoltaics, and will understand bonding/failure mechanisms. (Collaborations underway with Prof. Dauskardt, Prof. Salleo)

Key Publication:

"Enhanced water vapor blocking in transparent hybrid polymer-nanocrystal films", Eun Seon Cho, Christopher M. Evans, Emily C. Davidson, Megan L. Hoarfrost, Miguel A. Modestino, Rachel A. Segalman, and *Jeffrey J. Urban, *ACS Macro Lett.*, **4**, 70-74 (2015).