Noncrystallizable Molecular Glasses for Stable and Long-Lived OLED and Organic Electronics

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Abstract

Organic Light Emitting Diode Technology (OLED) is poised to challenge Light Emitting Diode (LED) and Liquid Crystal Display (LCD) in flat panel displays, flexible displays, and lighting applications. OLED display has an advantage over LCD with its high response speed, wide viewing angle, and high contrast in dark settings. There are, however, two major challenges slowing down OLED: production costs must decrease and device longevity needs to improve.[1, 2, and 3]

This presentation will introduce a new class of noncrystallizable charge transporting and/or electroluminescent materials designed to improve device stability and efficiency. We will report on the design, synthesis, and characterization of noncrystallizable electron-transporting, hole-transporting, bipolar charge-transporting, and luminescent small molecule materials. The concept behind this class of compounds and the reasons for their efficacy will be discussed.

Traditional thermal OLED production is too expensive. Solution processes for spin, roll-to-roll, slot die, or inkjet coating are required. The traditional small molecules used for thermal deposition tend to crystallize in solvents. OLED systems using polymeric materials (PLED) are being developed. Polymeric charge transport materials tend to have relatively low transport properties. Recently, there have been a lot of activities surrounding "molecular glasses" for solution smOLED processes (small molecules OLED).[4] *These molecular glasses are defined as "amorphous materials in the state of thermodynamic non-equilibrium, and hence, they tend to undergo structural relaxation, exhibiting well-defined glass temperature* T_g*'s. However they also tend to crystallize on heating above their* T_g*'s, frequently exhibiting polymorphism".*[5, 6] *With time, equilibrium will lead to crystallization of these materials. When that happens, the performance of the device is degraded, limiting longevity. An additional problem with current small molecule OLED materials is their solubility. Either solubility is limited or requires non-green solvents.*

Molecular Glasses, a division of Molaire Consulting LLC, is developing a new class of truly noncrystallizable amorphous small molecule organic electronics materials with high solubility in various green solvents.[7] *This new class of amorphous small molecule OLED materials is defined as mixtures of compatible molecules with an infinitely low crystallization rate under the most favorable conditions. They are essentially noncrystallizable with a large entropy of mixing values amenable to compatibility with a wide range of materials at a very high concentration.*

Molecular Glass Mixture Concept

Molecular glass mixture is not a new concept. Molaire introduced the concept back in 1985 in U.S. patents 4,499,165 and 4,626,361. The concept is fully described by Molaire & Johnson in "Organic Monomeric Glasses: A Novel Class of Materials."[8] As shown in Fig. 1, a polyfunctional organic nucleus is a common feature of all the molecules in the mixtures. The substituents are chosen to be different enough so that the rate of crystallization is infinitely low. However the substituents are similar enough so that all the molecules in the mixture are completely compatible. All the components of the mixture are synthesized in a single reaction. The challenge is to insure the purity of the glass mixture (by definition, recrystallization is not an option). Thus the following steps are followed:

1. Quantitative reactions (the reaction is near 100% complete);
2. No byproducts or byproducts that can be easily solubilized in water/other solvent and extracted efficiently;
3. Pre-purificating all starting materials by either recrystallization, sublimation, or distillation to purity level required for polycondensation reactions
4. Eliminating the transport of unwanted impurities from any of the starting materials to the produced amorphous material
5. Use of column chromatography when necessary

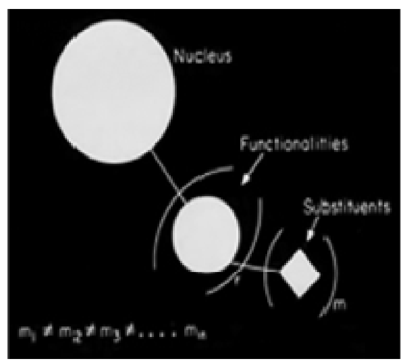

Figure 1

Important Attributes of Molecular Glass Mixtures

The molecular glass mixtures are designed to be noncrystallizable. This has been demonstrated by their use in the original Eastman Kodak 14-inch optical disc dye-binder media, the world's first 14-megapixel optical storage media[9] (with a 10-year lifetime warranty). However two other attributes contribute to the performance of the Kodak disc: the low melt viscosity of the glass mixture and its ability to solubilize high concentrations of additives. In the case of the Kodak dye-binder media, compatible molecular glass/dye compositions as high as 60 wt.% dye were achieved.[10, 11, 12] This ability to mix with other materials at a high concentration is a result of the large entropy of mixing of the glass mixture, an attribute that can be enhanced by controlling the number of components of the mixture[7].

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Author Biography

__Michel F. Molaire__ is CEO and founder of Molecular Glasses, a division of Molaire Consulting LLC. He received a BS (chemistry), M.S. (polymer science), and MBA from the University of Rochester. His experience includes polymer synthesis, photopolymerization, molecular glasses, optical recording materials, electrographic masters, photoreceptors, pigment dispersions, conductive coatings, castable polyurethane, image transfer materials, and dip coating technology. He holds 58 U.S. patents. Molaire is the recipient of Kodak's C.E.K. Mees Award for excellence in scientific research and reporting, an inductee to Kodak's Distinguished Inventor's Gallery, and an inductee to the African Scientific Institute Fellowship. He is a member of ACS, SPIE, and IS&T. He currently serves as a Board Member of both the IS&T and the Rochester Professional Consultants Network.